BEFORE THE OIL CONSERVATION COMMISSION
COMMENCING NOVEMBER 12, 2024

CASE NO. 23580

WILD EARTH GUARDIANS – PFAS RULEMAKING

PART 2

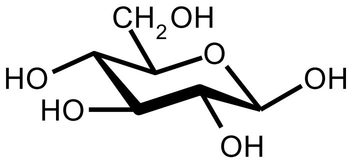
NMOGA
NEW MEXICO OIL AND GAS ASSOCIATION

NMOGA EXHIBIT D10.40
THROUGH NMOGA EXHIBIT E5.6

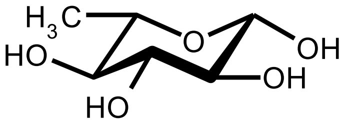
α (alpha), β (beta)

Stereodescriptors, used in a number of different ways.

1. Relative stereodescriptors used in carbohydrate nomenclature to describe the configuration at the anomeric carbon by relating it to the anomeric reference atom. For simple cases the anomeric reference atom is the same as the configurational reference atom. Thus in α-D-glucopyranose the reference atom is C-5 and the OH at C-1 is on the same side as the OH at C-5 in the Fischer projection.

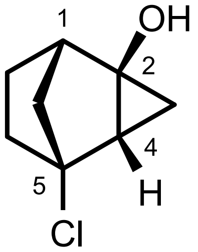


β-D-glucose



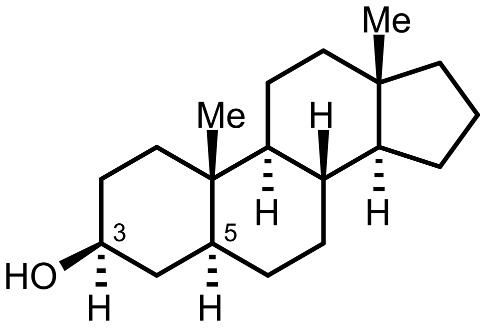
β-L-rhamnose

2. Relative stereodescriptors used by Chemical Abstracts Service to describe the configuration of a cyclic molecule (including suitable polycyclic systems) with several stereogenic centres whereby the α side of the reference plane is the side on which the substituent with CIP priority lies at the lowest numbered stereogenic centre. The other side is β.



tricyclo[3.2.1.0^{2,4}]octan-2-ol, 5-chloro, (1α,2α,4α,5β)-

3. Absolute stereodescriptors originally devised for steroid nomenclature. However in this sense it is only meaningful if there is an agreed absolute configuration and orientation of the structure so as to define the plane and which way up the molecule is represented. Substituents above the plane of the steroid are described as β and are shown as a solid line (▬ or ━); those below the plane are described as α and are shown by a broken line (⋯ or - - - -). The extension of this system to tetrapyrroles has been documented and it has been widely used elsewhere.



5α-androstan-3β-ol

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2197

See also:
PAC, 1989, *61*, 1783 *(Nomenclature of steroids (Recommendations 1989))* on page 1783
PAC, 1987, *59*, 779 *(Nomenclature of tetrapyrroles (Recommendations 1986))* on page 779

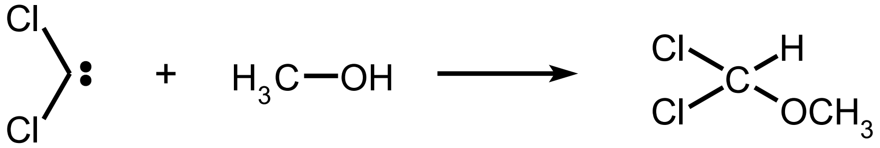
α- (β-, γ-) ray spectrometer

A measuring assembly incorporating a radiation detector and a pulse amplitude, used for determining the energy spectrum of α (β, γ) radiation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552

α-addition (alpha-addition)

A chemical reaction resulting in a single reaction product from two or three reacting chemical species, with formation of two new chemical bonds to the same atom in one of the reactant molecular entities. The synonymous term 1/1/addition is also used. For example:

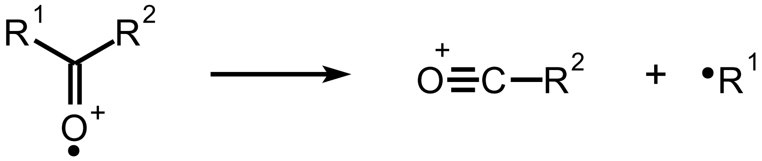


(This particular example can also be viewed as an insertion reaction). In inorganic chemistry such α-addition reactions, generally to a metallic central atom, are known as 'oxidative additions'. α-Addition is the reverse of α-elimination or 1/1/elimination.
See also: addition, elimination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1087

α-cleavage (alpha-cleavage)

1. (*in mass spectrometry*) The fission of a bond originating at an atom which is adjacent to one assumed to bear the charge; the definition of β-, γ-, cleavage then follows automatically. The process:



would thus be described as α-fission of a ketone with expulsion of a radical $R^{1\cdot}$. The carbon atoms of the radical $R^{1\cdot}$ are called the α-, β-, γ-carbons, starting with the atom nearest the functional group.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1558

2. (*in photochemistry*) Homolytic cleavage of a bond connecting an atom or group to an *excited chromophore*. Often applied to a bond connected to a carbonyl group, in which case it is called a Norrish type I photoreaction.
Note:
This reaction should be distinguished from an alpha-(α-)elimination.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 302

α-decay (alpha-decay)

Radioactive decay in which an alpha particle is emitted.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

α-effect

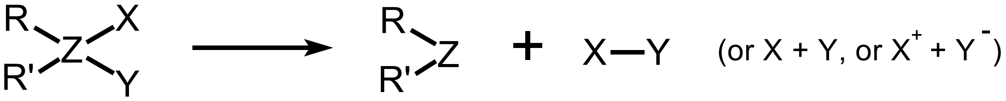
A positive deviation of an α-nucleophile (a nucleophile bearing an unshared pair of electrons on an atom adjacent to the nucleophilic site) from a Brønsted-type plot of $\log k_{\mathrm{nuc}}$ vs. $\mathrm{p}K_{\mathrm{a}}$ constructed for a series of related normal nucleophiles. More generally, it is the influence of the atom bearing a lone pair of electrons on the reactivity at the adjacent site.
See also: Brønsted relation

The use of the term has been extended to include the effect of any substituent on an adjacent reactive centre, for example in the case of the 'α-silicon effect'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1088

α-elimination

1. A transformation of the general type:



   where the central atom Z is commonly carbon. The reverse reaction is called α-addition.

   Source:
   PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1088
2. (*in photochemistry*) General term applied to a reaction by which a group attached to the alpha carbon of an *excited chromophore* is expelled either as an odd electron species or as an ionic species.
   Note:
   This reaction should be distinguished from an alpha-(α-)cleavage.

   Source:
   PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 302

α-expulsion

in photochemistry

A general reaction by which a group attached to the alpha carbon of an excited chromophore is expelled either as an odd electron species or as an anionic species. This reaction should be distinguished from an α- (alpha-) cleavage.

Source:
PAC, 1988, *60*, 1055 *(Glossary of terms used in photochemistry (Recommendations 1988))* on page 1059

α-oxo carbenes

Synonymous with acyl carbenes.
See also: keto carbenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

α-particle (alpha-particle)

Nucleus of the ^{4}He atom.

Source:
Green Book, 2nd ed., p. 93

'A' value

Also contains definition of: Winstein–Holness A value

The conformational preference of an equatorial compared to an axial substituent in a monosubstituted cyclohexane. This steric substituent parameter equals $\Delta_r G^0$ in $\mathrm{kcal\ mol^{-1}}$ for the equatorial to axial equilibration on cyclohexane. The values are also known as 'Winstein–Holness' A values.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1087

ab initio quantum mechanical methods

Synonym: non-empirical quantum mechanical methods

Methods of quantum mechanical calculations independent of any experiment other than the determination of fundamental constants. The methods are based on the use of the full Schroedinger equation to treat all the electrons of a chemical system. In practice, approximations are necessary to restrict the complexity of the electronic wavefunction and to make its calculation possible.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1921
This definition supersedes an earlier definition of *ab initio* calculations.

abatement

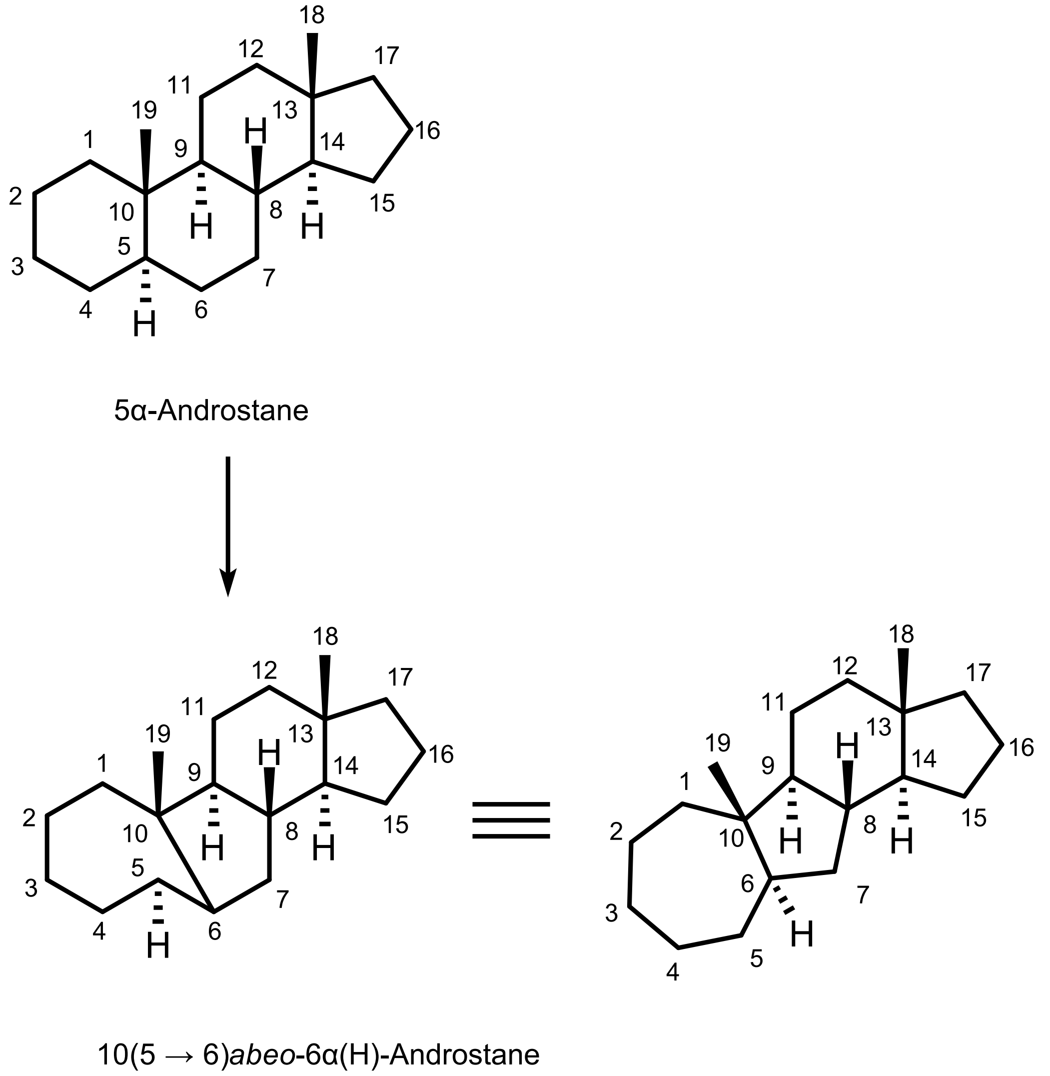
in atmospheric chemistry

Action taken to reduce air pollution which involves the use of control equipment or some new process. This refers to a reduction or lessening as opposed to elimination of a type of discharge or pollutant.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169

abeo-

Bond migration, i.e. the formal transfer of one end of a skeletal bond to another position, with a compensating transfer of a hydrogen atom, can be indicated by a prefix of the form '$x(y \rightarrow z)$*abeo-*'. The prefix is compiled as follows: a numeral denoting the stationary (unchanged) end of the migrating bond (x) is followed by parentheses enclosing the locant denoting the original position (y) from which the other end of this bond has migrated, an arrow, and the locant (*z*) denoting the new position to which the bond has moved. The closing parenthesis is followed by the italicized prefix *abeo*-(Latin: I go away) to indicate bond migration. The original numbering is retained for the new compound and is used for the numbers *x*, *y* and *z*. It is always necessary to specify the resulting stereochemistry.



5α-Androstane

10(5 → 6)*abeo*-6α(H)-Androstane

Source:
Blue Book (Guide), p. 31

abiotic

Synonym: abiological

Not associated with living organisms. Synonymous with abiological.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2007

abiotic transformation

Process in which a substance in the environment is modified by non-biological mechanisms.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2007

absolute activation analysis

A kind of activation analysis in which the elemental concentrations in the material are calculated from known nuclear constants, irradiation and measurement parameters, rather than by comparing with known standards.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515

absolute activity, λ

The exponential of the ratio of the chemical potential, μ, to $R\,T$ where R is the gas constant and T the thermodynamic temperature, $\lambda = \mathrm{e}^{\frac{\mu}{R\,T}}$.

Source:
Green Book, 2nd ed., p. 40

See also:
PAC, 1984, *56*, 567 *(Physicochemical quantities and units in clinical chemistry with special emphasis on activities and activity coefficients (Recommendations 1983))* on page 569
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 959

absolute configuration

The spatial arrangement of the atoms of a chiral molecular entity (or group) and its stereochemical description e.g. *R* or *S*.
See also: relative configuration, α (alpha), β (beta)

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2197

See also:
Blue Book, p. 474

absolute counting

in radioanalytical chemistry

A measurement under such well-defined conditions that the activity of a sample can be derived directly from the observed counting rate.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517

absolute electrode potential

The electrode potential of a metal measured with respect to a universal reference system (not including any additional metal/solution interface).

Source:
PAC, 1986, *58*, 955 *(The absolute electrode potential: an explanatory note (Recommendations 1986))* on page 957

absolute full energy peak efficiency

Of a radiation spectrometer, the counting efficiency when considering only the events recorded in the full energy peak.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

absolute lethal concentration (LC_{100})

Lowest concentration of a substance in an environmental medium which kills 100% of test organisms or species under defined conditions. This value is dependent on the number of organisms used in its assessment.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2007

absolute lethal dose (LD_{100})

Lowest amount of a substance which kills 100% of test animals under defined conditions. This value is dependent on the number of organisms used in its assessment.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2007

absolute photopeak efficiency

Of a γ-ray spectrometer, the counting efficiency when only the events recorded in the photopeak are considered.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

absolute preconcentration

in trace analysis

An operation (process) as the result of which microcomponents are transferred from the sample of larger mass into the sample of smaller mass, so that the concentration of the microcomponents is increased. Examples include the decrease in solvent volume during distillation or evaporation, and the transfer of microcomponents from an aqueous solution into a smaller volume of organic solvent by extraction.

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1197

absorbance, A

Logarithm of the ratio of incident to transmitted radiant power through a sample (excluding the effects on cell walls). Depending on the base of the logarithm a decadic and Napierian absorbance are used. Symbols: A, A_{10}, A_e. This quantity is sometimes called extinction, although the term extinction, better called attenuance, is reserved for the quantity which takes into account the effects of luminescence and scattering as well.

Source:
Green Book, 2nd ed., p. 32

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2226
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169

absorbance matching

in spectrochemical analysis

A procedure where the concentration of a known analyte may be determined by diluting the sample with solvent until the absorbance matches the absorbance of the analyte in the reference cell. This method is particularly useful if the Beer-Lambert law does not hold.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1456

absorbed dose

of a substance

Amount of a substance absorbed into an organism or into organs and tissues of interest.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2007

absorbed dose, *D*

of radiation

Energy imparted to matter by ionizing radiation in a suitable small element of volume divided by the mass of that element of volume.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 959
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2007
Orange Book, p. 220

absorbed electron coefficient

in in situ microanalysis

Number of absorbed electrons per primary electron.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2026

absorbed electrons

in in situ microanalysis

The (excess) electrons present in a specimen under electron bombardment which are led to ground and measured as specimen current. The number of absorbed electrons per unit time (or the specimen current), equals the number of primary electrons minus the number of back scattered, secondary and transmitted electrons per unit time. Therefore the fraction of electrons being absorbed depends on many parameters, including the composition and thickness of the specimen, the primary electron energy, the electron incidence angle and local electrostatic fields when present.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2026

absorbed (spectral) photon flux density

Number of photons of a particular wavelength per time interval (spectral photon flux, number basis, $q_{\mathrm{p},\lambda}$, or spectral photon flux, amount basis, $q_{n,\mathrm{p},\lambda}$) absorbed by a system per volume, V. On number basis, SI unit is $\mathrm{s^{-1}\ m^{-4}}$ common unit is $\mathrm{s^{-1}\ cm^{-3}\ nm^{-1}}$ On amount basis, SI unit is $\mathrm{mol\ s^{-1}\ m^{-4}}$ common unit is $\mathrm{einstein\ s^{-1}\ cm^{-3}\ nm^{-1}}$.

Notes:

1. Mathematical expression: $\frac{q^0_{\mathrm{p},\lambda}\,[1-10^{-A(\lambda)}]}{V}$ on number basis, $\frac{q^0_{n,\mathrm{p},\lambda}\,[1-10^{-A(\lambda)}]}{V}$ on amount basis, where $A(\lambda)$ is the absorbance at wavelength λ and superscript 0 (zero) indicates incident photons.
2. Absorbed spectral photon flux density (number basis or amount basis) should be used in the denominator when calculating a differential quantum yield and using in the numerator the rate of change of the number concentration, $\frac{\mathrm{d}C}{\mathrm{d}t}$ or the rate of change of the amount concentration, $\frac{\mathrm{d}c}{\mathrm{d}t}$, respectively.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 297

absorbed (spectral) radiant power density

Spectral radiant energy per time interval (spectral radiant power, P_λ) absorbed by a system per volume, V. SI unit is $\mathrm{W\ m^{-4}}$; common unit is $\mathrm{W\ cm^{-3}\ nm^{-1}}$.

Note:

Mathematical expression: $\frac{P^0_\lambda\,[1-10^{-A(\lambda)}]}{V}$, where $A(\lambda)$ is the absorbance at wavelength λ and superscript 0 (zero) indicates incident radiant power.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 297

absorber

1. A device used commonly for sampling by absorption in which a gaseous or liquid material is removed from another gas or liquid by selective absorption; these include: scrubber, impinger, packed column, spray chamber, etc.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169

2. A substance used to absorb energy from any type of radiation.

   Source:
   PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1534

absorptance, α

Ratio of the absorbed to the incident radiant power. Also called absorption factor. When $\alpha \leq 1$, $\alpha \approx A_e$, where A_e is the Napierian absorbance.

Source:
Green Book, 2nd ed., p. 32

See also:
PAC, 1985, *57*, 105 *(Names, symbols, definitions and units of quantities in optical spectroscopy (Recommendations 1984))* on page 114
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 959
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2226

absorption

1. The process of one material (absorbate) being retained by another (absorbent); this may be the physical solution of a gas, liquid, or solid in a liquid, attachment of molecules of a gas, vapour, liquid, or dissolved substance to a solid surface by physical forces, etc. In spectrophotometry, absorption of light at characteristic wavelengths or bands of wavelengths is used to identify the chemical nature of molecules, atoms or ions and to measure the concentrations of these species.

   Source:
   PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169
2. A phenomenon in which radiation transfers to matter which it traverses some of or all its energy.

   Source:
   PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1534
   PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2226

absorption coefficient

Linear decadic (a, K) and Napierian absorption coefficients (α) are equal to the corresponding absorbances divided by the optical path length through the sample. The molar absorption coefficients (decadic ε, Napierian κ) are the linear absorption coefficients divided by the amount concentration.

Source:
Green Book, 2nd ed., p. 32

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2226
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 959

absorption coefficient

in biology

Ratio of the absorbed quantity (uptake) of a substance to the administered quantity (intake).

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1036

absorption cross-section, σ

Molar Napierian absorption coefficient divided by the Avogadro constant. When integrated against the logarithm of wavenumber (or frequency) it is called the integrated absorption cross-section.

Source:
Green Book, 2nd ed., p. 32
Green Book, 2nd ed., p. 33

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2226

absorption factor

See: absorptance

Source:
Green Book, 2nd ed., p. 32
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 960

absorption intensity

Differently defined physical quantities describing the absorption of radiation by a sample.

Source:
Green Book, 2nd ed., p. 32
Green Book, 2nd ed., p. 33

absorption line

A narrow range of wavelengths in which a substance absorbs light; a series of discrete absorption lines can be used as an unambiguous identification for many relatively simple chemical species.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169

absorption pathlength

of a sample cell

The length of the radiation path through the absorbing medium; it is equal to the cell path length, l, in the case of single-pass cells at normal incidence of radiation.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1453

absorption spectrum

The wavelength dependence of the absorption cross-section (or absorption coefficient); usually represented as a plot of absorption cross-section versus wavelength λ (or $\frac{1}{\lambda}$) of the light.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169

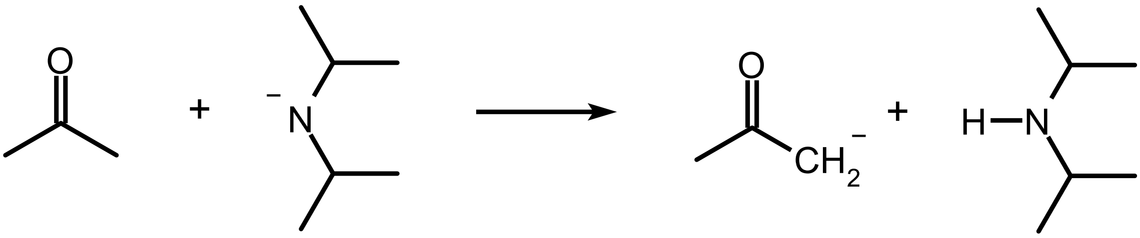
absorptivity [obsolete]

Absorptance divided by the optical path length. For very low attenuance it approximates the absorption coefficient [within the approximation $(1 - \mathrm{e}^{-A}) \sim A$]. The use of this term is not recommended.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2227

abstraction

A chemical reaction or transformation, the main feature of which is the bimolecular removal of an atom (neutral or charged) from a molecular entity. For example:



(proton abstraction from acetone)

$$CH_4 + {}^\bullet Cl \longrightarrow {}^\bullet CH_3 + HCl$$

(hydrogen abstraction from methane)
See: detachment

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

abstraction process

Also contains definition of: extraction process *in catalysis*

in catalysis

In abstraction and extraction processes, an adsorptive or adsorbate species extracts an adsorbed atom or a lattice atom respectively. Abstraction process:

$$^*H + H(g) \longrightarrow {}^* + H_2(g)$$

Extraction process:

$$O_S^{2-} + CO(g) \longrightarrow 2e^- + CO_2(g)$$

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 85

abundance sensitivity

in mass spectrometry

The ratio of the maximum ion current recorded at a mass m to the ion current arising from the same species recorded at an adjacent mass ($m \pm 1$).

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1554

ac

See: torsion angle

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2197

accelerating voltage (high voltage, V) scan

in mass spectrometry

This is an alternative method of producing a momentum (mass) spectrum in magnetic deflection instruments by varying the accelerating voltage. This scan can also be used, in conjunction with a fixed radial electric field, to produce an ion kinetic energy spectrum.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

acceleration, a

Vector quantity equal to the derivative of velocity with respect to time. For the acceleration of free fall the symbol g is used.

Source:
Green Book, 2nd ed., p. 11
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 960

acceleration energy

in in situ microanalysis

See: excitation energy *in in situ microanalysis*

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2027

acceleration of free fall, g

Acceleration of free fall in vacuum due to gravity. Also called acceleration due to gravity.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 960

accelerator

in solvent extraction

Synonymous with catalyst.
See: catalyst, kinetic synergist, modifier

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2380

acceptable daily intake (ADI)

Estimate by JECFA of the amount of a food additive, expressed on a body-weight basis, that can be ingested daily over a lifetime without appreciable health risk.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1036
This definition supersedes an earlier definition of acceptable daily intake (ADI).

acceptor number (AN)

A quantitative measure of Lewis acidity.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

accommodation coefficient

A measure of the efficiency of capture of molecules or atoms which collide with aerosol particles, cloud droplets, etc. The accommodation coefficient is the fraction of the collisions which result in the capture of the molecules (atoms, radicals, etc.) by the particle, cloud droplet, etc.; fraction of colliding molecules which are not reflected but which enter the surface of an aqueous aerosol. Synonymous with sticking coefficient.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169

accretion

in atmospheric chemistry

The process by which aerosols grow in size by external addition of various chemical species; a form of agglomeration.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169

accuracy

of a measuring instrument

Ability of a measuring instrument to give responses close to a true value.

Source:
VIM
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

accuracy

of measurement

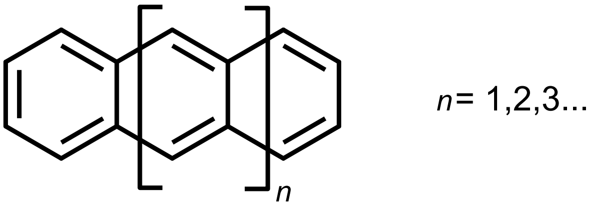
Closeness of the agreement between the result of a measurement and a true value of the measurand.
Notes:

1. Accuracy is a qualitative concept.
2. The term precision should not be used for accuracy.

Source:
VIM
Orange Book, p. 6
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2170
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 598

acenes

Polycyclic aromatic hydrocarbons consisting of fused benzene rings in a rectilinear arrangement.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1310

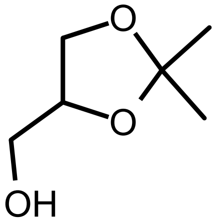
acetals

Compounds having the structure $R_2C(OR')_2$ (R' ≠ H) and thus diethers of geminal diols. Originally, the term was confined to derivatives of aldehydes (one R = H), but it now applies equally to derivatives of ketones (neither R = H). Mixed acetals have different R' groups.
See also: acetonides, ketals, acylals, hemiacetals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1310

acetonides

Cyclic acetals derived from acetone and diols, usually vicinal diols, or polyhydroxy compounds. E.g.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1311

acetylene black

A special type of carbon black formed by an exothermic decomposition of acetylene. It is characterized by the highest degree of aggregation and crystalline orientation when compared with all types of carbon black.
Note:
Acetylene black must not be confused with the carbon black produced as a by-product during the production of acetylene in the electric arc process.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 476

acetylenes

Acyclic (branched or unbranched) and cyclic (with or without side chain) hydrocarbons having one or more carbon–carbon triple bonds.

See also: alkynes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1311

acetylides

Compounds arising by replacement of one or both hydrogen atoms of acetylene (ethyne) by a metal or other cationic group. E.g. NaC≡CH monosodium acetylide. By extension, analogous compounds derived from terminal acetylenes, RC≡CH.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1311

Acheson graphite

A synthetic graphite made by the Acheson process.
Note:
Reference to Acheson in combination with synthetic graphite honours the inventor of the first technical graphitization. Today the term Acheson graphite, however, is of historical interest only because it no longer covers the plurality of synthetic graphite.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 476

achiral

See: chirality

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2197
Blue Book, p. 479

aci-nitro compounds

A class name for hydrocarbylideneazinic acids, $R_2C{=}N^+(–O^-)OH$. The use of *aci*-nitro as a prefix in systematic nomenclature to name specific compounds is abandoned.
See also: azinic acids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

acid

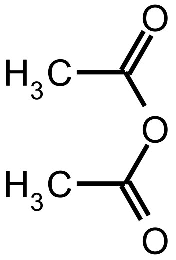
A molecular entity or chemical species capable of donating a hydron (proton) (see Brønsted acid) or capable of forming a covalent bond with an electron pair (see Lewis acid).
See also: hard acid, carboxylic acids, oxoacids, sulfonic acids

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

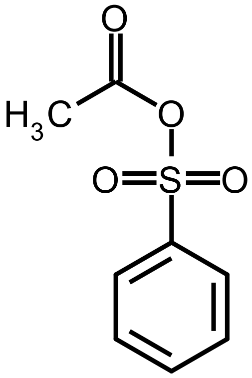
See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2170

acid anhydrides

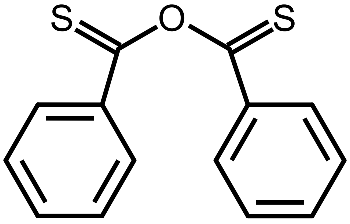
Compounds consisting of two acyl groups bonded to the same oxygen atom acyl-O-acyl. Symmetric and mixed anhydrides have identical and different acyl groups, respectively. E.g.



acetic anhydride,



acetic benzenesulfonic anhydride,



(thiobenzoic) anhydride.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1311

acid deposition

in atmospheric chemistry

The acids deposited by transfer from the atmosphere either by precipitation (rain, fog, snow, etc.), called wet deposition, or by direct transfer to the surface of the earth induced by the flow of acid-containing air masses over the earth's surface, called dry deposition.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2170

acid rain

in atmospheric chemistry

Rain with pH values < about 5; commonly results from acids formed from pollutants. 'Pure' rain water equilibrated with atmospheric CO_2 and naturally occurring acids in relatively clean air usually has a $\mathrm{pH} > 5$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2170

acid-labile sulfur

Refers to sulfido ligands, e.g., the bridging ligands in iron-sulfur proteins, which are released as H_2S at acid pH.
See also: ferredoxin

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1254

acidity

1. Of a compound: For Brønsted acids the tendency of a compound to act as a hydron donor. It can be quantitatively expressed by the acid dissociation constant of the compound in water or some other specified medium. For Lewis acids it relates to the association constants of Lewis adducts and π adducts.
2. Of a medium: The use of the term is mainly restricted to a medium containing Brønsted acids, where it means the tendency of the medium to hydronate a specific reference base. It is quantitatively expressed by the appropriate acidity function.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

acidity constant

The equilibrium constant $K_{\mathrm{a}n}$ for splitting off the *n*th proton from a charged or uncharged acid, to be defined. One may write K_{a} for $K_{\mathrm{a}1}$.

Source:
Orange Book, p. 13

acidity function

Also contains definitions of: basicity function, Hammett acidity function

Any function that measures the thermodynamic hydron-donating or -accepting ability of a solvent system, or a closely related thermodynamic property, such as the tendency of the lyate ion of the solvent system to form Lewis adducts. (The term 'basicity function' is not in common use in connection with basic solutions.) Acidity functions are not unique properties of the solvent system alone, but depend on the solute (or family of closely related solutes) with respect to which the thermodynamic tendency is measured. Commonly used acidity functions refer to concentrated acidic or basic solutions. Acidity functions are usually established over a range of composition of such a system by UV/VIS spectrophotometric or NMR measurements of the degree of hydronation (protonation or Lewis adduct formation) for the members of a series of structurally similar indicator bases (or acids) of different strength: the best known of these functions is the Hammett acidity function H_0 (for uncharged indicator bases that are primary aromatic amines).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

acidosis

Pathological condition in which the hydrogen ion substance concentration of body fluids is above normal and hence the pH of blood falls below the reference interval.
See also: alkalosis

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2009

acid–base indicator

An acid or base which exhibits a colour change on neutralization by the basic or acidic titrant at or near the equivalence point of a titration.

Source:
Orange Book, p. 48

actinic

Applied or referred to actinism.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 300

actinic flux S_λ

The quantity of light available to molecules at a particular point in the atmosphere and which, on absorption, drives photochemical processes in the atmosphere. It is calculated by integrating the spectral radiance $L(\lambda,\ \theta,\ \phi)$ overall directions of incidence of the light, $E(\lambda) = \int\limits_{\theta}\int\limits_{\varphi} L(\lambda,\ \theta,\ \varphi) \cos\theta \sin\theta \mathrm{d}\theta\mathrm{d}\varphi$. If the radiance is expressed in $\mathrm{J\ m^{-2}\ s^{-1}\ st^{-1}\ nm^{-1}}$ and hc/λ is the energy per quantum of light of wavelength λ, the actinic flux has units of $\mathrm{quanta\ cm^{-2}\ s^{-1}\ nm^{-1}}$. This important quantity is one of the terms required in the calculation of *j*-values, the first order rate coefficients for photochemical processes in the sunlight-absorbing, trace gases in the atmosphere. The actinic flux is determined by the solar radiation entering the atmosphere and by any changes in this due to atmospheric gases and particles (e.g. Rayleigh scattering absorption by stratospheric ozone, scattering and absorption by aerosols and clouds), and reflections from the ground. It is therefore dependent on the wavelength of the light, on the altitude and on specific local environmental conditions. The actinic flux has borne many names (e.g. flux, flux density, beam irradiance actinic irradiance, integrated intensity) which has caused some confusion. It is important to distinguish the actinic flux from the spectral irradiance, which refers to energy arrival on a flat surface having fixed spatial orientation ($\mathrm{J\ m^{-2}\ nm^{-1}}$) given by:

$$E(\lambda) = \int\limits_{\theta}\int\limits_{\varphi} L(\lambda,\ \theta,\ \varphi) \cos\theta \sin\theta \mathrm{d}\theta\mathrm{d}\varphi.$$

The actinic flux does not refer to any specific orientation because molecules are oriented randomly in the atmosphere. This distinction is of practical relevance: the actinic flux (and therefore a *j*-value) near a brightly reflecting surface (e.g. over snow or above a thick cloud) can be a factor of three higher than that near a non-reflecting surface. The more descriptive name of spectral spheradiance is suggested for the quantity herein called actinic flux.
See also: flux density, photon

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2170

actinism

Chemical changes on living and non-living materials caused by optical radiation.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 300

actinometer

A chemical system or physical device which determines the number of photons in a beam integrally or per unit time. This name is commonly applied to devices used in the ultraviolet and visible wavelength ranges. For example, solutions of iron(III) oxalate can be used as a chemical actinometer, while bolometers, thermopiles, and photodiodes are physical devices giving a reading that can be correlated to the number of photons detected.
See also: chemical actinometer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2227

action spectrum

A plot of a relative biological or chemical photoresponse ($= \Delta y$) per number of incident photons against wavelength or energy of radiation under the same radiant power of light. This form of presentation is frequently used in the studies of biological or solid state systems, where the nature of the absorbing species is unknown. This type of action spectrum is sometimes called spectral responsivity or sensitivity spectrum. The precise action spectrum is a plot of the spectral or quantum) effectiveness. By contrast, a plot of the biological or chemical change or response per absorbed photon (quantum efficiency) versus wavelength is the efficiency spectrum.
See also: excitation spectrum, efficiency spectrum

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2227

activated adsorption process

If the temperature coefficient of the rate of adsorption is substantial, an adsorption process is said to be activated (i.e. to have a significant activation energy). In this case, the sticking coefficient is small. In general, the activation energy of activated adsorption is a function of coverage and it usually increases with increasing coverage.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

activated carbon

A porous carbon material, a char which has been subjected to reaction with gases, sometimes with the addition of chemicals, e.g. $ZnCl_2$, before, during or after carbonization in order to increase its adsorptive properties.
Note:
Activated carbons have a large adsorption capacity, preferably for small molecules, and are used for purification of liquids and gases. By controlling the process of carbonization and activation, a variety of active carbons having different porosity can be obtained. Activated carbons are used mainly in granular and powdered forms, but can also be produced in textile form by controlled carbonization and activation of textile fibres. Other terms used in the literature: active carbons, active charcoals.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 476

activated charcoal

A traditional term for activated carbon.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 476

activated complex

An activated complex, often characterized by the superscript ‡, is defined as that assembly of atoms which corresponds to an arbitrary infinitesimally small region at or near the col (saddle point) of a potential energy surface.
See also: transition state

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

See also:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2292
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 150

activation

Also contains definition of: degree of activation

This word is used in different senses:

1. Input of external energy into a chemical system is said to bring about activation of the system.
2. An added substance that increases the rate of a catalysed reaction is known as an activator, and the effect is called activation. The degree of activation ε_a is defined by:

$$\varepsilon_a = \frac{v - v_0}{v_0} = \frac{v}{v_0} - 1$$

where v_0 is the rate of the catalysed reaction in the absence of the activator and v is the rate of the catalysed reaction in the presence of the activator

3. When some of the energy required for a reaction to occur is provided by a previous exothermic chemical reaction there is said to be chemical activation.

See: chemical activation, catalysis
See also: activator, inhibition

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 151

activation analysis (nuclear)

A kind of elemental or isotopic analysis based on the measurement of characteristic radiation from nuclides formed directly or indirectly by activation of the test portion. In general, a specification is added of the type of the incident radiation (e.g. neutron, photon) and its energy (e.g. thermal, fast).

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515
Orange Book, p. 210

activation cross-section

The cross-section for the formation of a radionuclide by a specified reaction.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517
Orange Book, p. 217

activation energy (Arrhenius activation energy)

An empirical parameter characterizing the exponential temperature dependence of the rate coefficient, k, $E_a = R\,T^2\,\frac{\mathrm{d}(\ln k)}{\mathrm{d}T}$, where R is the gas constant and T the thermodynamic temperature. The term is also used for threshold energies in electronic potential surfaces, in which case the term requires careful definition.

Source:
Green Book, 2nd ed., p. 55

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 151

PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2294
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

activation

in electrochemical corrosion

The process of transition from the passive to the active state by removal of the passivating film. A necessary condition for activation is an electrode potential negative to the equilibrium potential of formation of the passivating film. Activation is achieved by cathodic currents, by a reduced substance in the adjacent solution, or by contact with an electronic conductor having a suitably negative corrosion potential.
See also: passive state, active state

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

activation

in radiochemistry

The process of inducing radioactivity by irradiation. In general, a specification is added of the type of incident radiation (e.g. nuclear, neutron, photon) or its energy (e.g. thermal, fast).

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515

activation reaction

Process leading from the reactants to the formation of an activated complex or transition state.

Source:
Physical Chemistry Division, unpublished

activator

Also contains definition of: enzyme activator

A substance, other than the catalyst or one of the substrates, that increases the rate of a catalysed reaction without itself being consumed; the process is called activation. An activator of an enzyme-catalysed reaction may be called enzyme activator, if it acts by binding to the enzyme.
See also: effector

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2292

active centre

See: active site

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 77

See also:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 145

active medium

See: laser

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1915

active metal

in electrochemical corrosion

A metal corroding in the active state.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

active site

in heterogeneous catalysis

The term is often applied to those sites for adsorption which are the effective sites for a particular heterogeneous catalytic reaction. The terms active site and active centre are often used as synonyms, but active centre may also be used to describe an ensemble of sites at which a catalytic reaction takes place.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 77

See also:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 145

active solid

A porous solid with adsorptive properties by means of which chromatographic separations may be achieved. The separations resulting from this action follow laws different from those deriving from the partitioning action of the liquid phase.

Source:
Orange Book, p. 98

active species

See: laser

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1915

active state

in electrochemical corrosion

Corrosion in the active state occurs by direct transfer (which may involve one or several steps) of metal ions from the metallic phase to the adjacent electrolyte. The corrosion current of an active metal usually increases when the electrode potential is made more positive, other conditions remaining constant.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

active transport

in biology

The carriage of a solute across a biological membrane from low to high concentration which requires the expenditure of (metabolic) energy.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 145

activity

See: activity (relative activity)

Source:
Green Book, 2nd ed., p. 49
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 989

activity, *A*

Synonyms: decay rate
of a radioactive material

, disintegration rate
of a radioactive material

of a radioactive material

The number of nuclear decays occurring in a given quantity of material in a small time interval, divided by that time interval. Often, this term is referred to as absolute activity. Symbol $A = -\frac{\mathrm{d}N}{\mathrm{d}t}$. Synonymous with disintegration rate or decay rate.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515
Green Book, 2nd ed., p. 22
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 960

activity coefficient, *f*, *γ*

The activity coefficient f_B of a substance B in a liquid or solid mixture containing mole fractions x_B, x_C, ... of the substances B, C, ... is a dimensionless quantity defined in terms of the chemical potential μ_B of B in the mixture by:

$$R\,T \ln(x_\mathrm{B}\, f_\mathrm{B}) = \mu_\mathrm{B}(\mathrm{cd},\, T,\, P,\, x) - \mu_\mathrm{B}^{*}(\mathrm{cd},\, T,\, p)$$

where x denotes the set of mole fractions x_B, x_C, ... The activity coefficient γ_B of a solute B in a solution (especially a dilute liquid solution) containing molalities m_B, m_C, ... of solutes B, C, ... in a solvent A is a dimensionless quantity defined in terms of the chemical potential μ_B by:

$$R\,T \ln\left(\frac{m_\mathrm{B}\,\gamma_\mathrm{B}}{m^{\ominus}}\right) = \mu_\mathrm{B} - \left\{\mu_\mathrm{B} - R\,T \ln\left(\frac{m_\mathrm{B}}{m^{\ominus}}\right)\right\}^{\infty}$$

Source:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 543
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 546
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2171
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 960

activity (relative activity), *a*

Defined by the equation

$$a = \mathrm{e}^{\frac{\mu-\mu^0}{RT}}$$

where R is the gas constant, T the thermodynamic temperature, μ the chemical potential and μ^0 the standard chemical potential the definition of which depends on the choice of the standard state.
See also: absolute activity

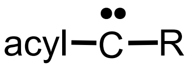
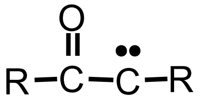
Source:
Green Book, 2nd ed., p. 49
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 989

acute toxicity

1. Adverse effects of finite duration occurring within a short time (up to 14 d) after administration of a single dose (or exposure to a given concentration) of a test substance or after multiple doses (exposures), usually within 24 h of a starting point (which may be exposure to the toxicant, or loss of reserve capacity, or developmental change, *etc.*)
2. Ability of a substance to cause adverse effects within a short time of dosing or exposure.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1037

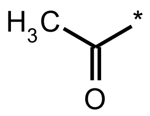
acyl carbenes

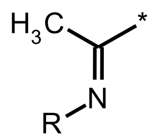
Any compound  $\mathrm{acyl{-}\ddot{C}{-}R}$. In organic chemistry, an unspecified acyl carbene is commonly a carboxylic acyl carbene,  $\mathrm{R{-}\overset{\overset{O}{\|}}{C}{-}\ddot{C}{-}R}$.

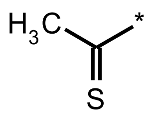
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1311

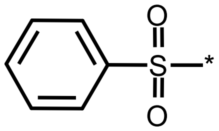
acyl groups

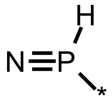
Groups formed by removing one or more hydroxy groups from oxoacids that have the general structure $R_kE(=O)_l(OH)_m$ ($1 \neq 0$), and replacement analogues of such acyl groups. In organic chemistry an unspecified acyl group is commonly a carboxylic acyl group. E.g.

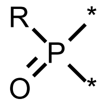








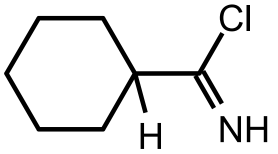




Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1311

acyl halides

Compounds consisting of an acyl group bonded to halogen, e.g. $CH_3S(=O)_2Cl$, methanesulfonyl chloride; CH_3COCl , acetyl chloride; cyclohexanecarboximidoyl chloride,



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1311

acyl shift (1,2-, 1,3-, photochemical)

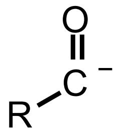
Photochemical process with skeletal isomerization by shift of an acyl group from position 1 to position 2 or 3.
See also: aza-di-π-methane rearrangement, di-π-methane rearrangement, di-π-silane rearrangement, oxa-di-π-methane rearrangement, photo-Fries rearrangement

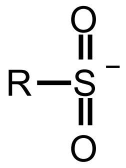
Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 301

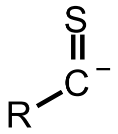
acyl species

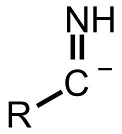
Also contains definitions of: acyl anions, acyl cations, acyl radicals, acylium ions

Acyl intermediates include acyl anions, acyl radicals and acyl cations (synonym acylium ions) which are formally derived from oxoacids $R_kE(=O)_l(OH)_m$ ($l \neq 0$) by removal of a hydroxyl cation HO^+ , a hydroxyl radical $HO^\cdot$ or a hydroxyl anion HO^- , respectively, and replacement analogues of such intermediates. Acyl anions, radicals and cations can formally be represented by canonical forms having a negative charge, an unpaired electron or a positive charge on the acid-generating element of the oxoacid. Acyl anions. E.g.

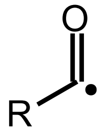


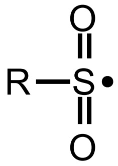




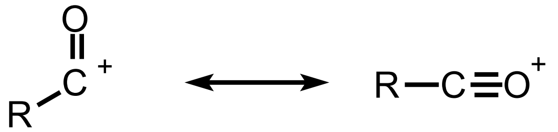


Acyl radicals. E.g.





Acyl cations. E.g.

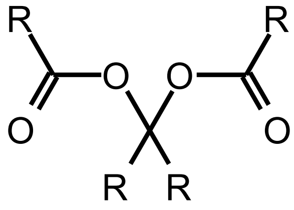


See also: acyl groups

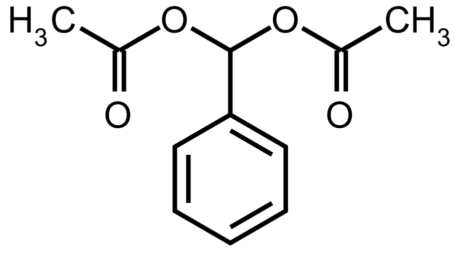
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

acylals

Diesters of geminal diols; i.e.



E.g. benzylidene diacetate:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1311

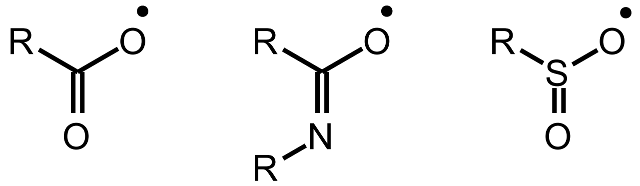
acyloins

α-Hydroxy ketones, RCH(OH)C(=O)R . So named from the fact that they are formally derived from reductive coupling of carboxylic acyl groups.
See also: ketones

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

acyloxyl radicals

Oxygen-centered radicals consisting of an acyl radical bonded to an oxygen atom. E.g.



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Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

addend

See: addition reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

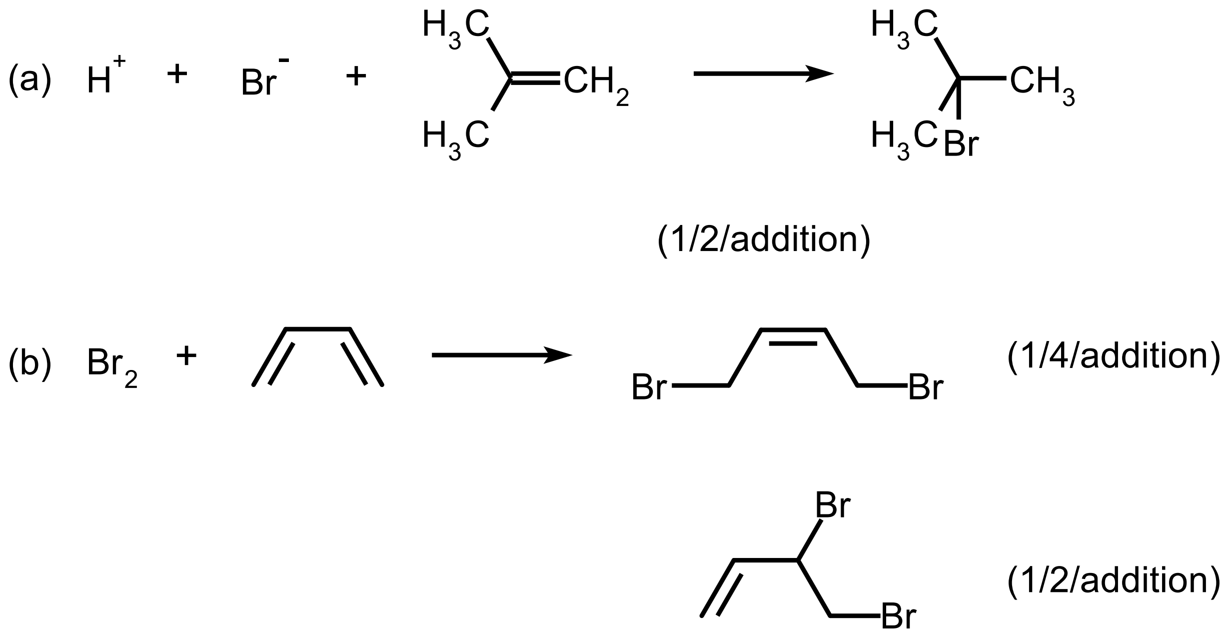
addition

1. Refers to addition reaction or addition transformation.
2. Loosely, the formation of an adduct. (For an example, see Lewis acid.)
3. Loosely, any association or attachment.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

addition reaction

A chemical reaction of two or more reacting molecular entities, resulting in a single reaction product containing all atoms of all components, with formation of two chemical bonds and a net reduction in bond multiplicity in at least one of the reactants. The reverse process is called an elimination reaction. The addition may occur at only one site (α-addition, 1/1/addition), at two adjacent sites (1/2/addition) or at two non-adjacent sites (1/3/- or 1/4/addition, etc.). For example:



If the reagent or the source of the addends of an addition are not specified, then it is called an addition transformation.

See also: addition, α-addition, cheletropic reaction, cycloaddition

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

additive

A substance added to a sample for any of a variety of purposes.

Source:
Orange Book, p. 159

additive name

1. The formal assembly of names for the components of a compound without loss of atoms or groups of atoms from any component.
2. The addition or attachment of atoms or groups of atoms.

Source:
Blue Book (Guide), p. 16

additivity

of mass spectra

The process by which each chemical species present in the ion source at a certain partial pressure makes a contribution to the total mass spectrum which is the same as that which it would give if that chemical species alone were present in the ion source at a pressure equal to this certain partial pressure.

Source:
Orange Book, p. 206

additivity principle

The hypothesis that each of several structural features of a molecular entity makes a separate and additive contribution to a property of the substance concerned. More specifically, it is the hypothesis that each of the several substituent groups in a parent molecule makes a separate and additive contribution to the standard Gibbs energy change (or Gibbs energy of activation) corresponding to a particular equilibrium (or rate of reaction).
See also: transferability

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1081

adduct

A new chemical species AB, each molecular entity of which is formed by direct combination of two separate molecular entities A and B in such a way that there is change in connectivity, but no loss, of atoms within the moieties A and B. Stoichiometries other than 1:1 are also possible, e.g. a bis-adduct (2:1). An intramolecular adduct can be formed when A and B are groups contained within the same molecular entity. This is a general term which, whenever appropriate, should be used in preference to the less explicit term complex. It is also used specifically for products of an addition reaction. For examples, see Lewis adduct, Meisenheimer adduct, π-adduct.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1082

adduct ion

in mass spectrometry

An ion formed by interaction of two species, usually an ion and a molecule, and often within the ion source, to form an ion containing all the constituent atoms of one species as well as an additional atom or atoms.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

adhesional wetting

A process in which an adhesional joint is formed between two phases.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 597

adiabatic

Also contains definition of: nonadiabatic

This word is used with various different meanings, and when it is used it should be defined. In thermodynamics 'adiabatic' is used in a macroscopic sense to refer to a process occurring in a thermally insulated system, so that there is no flow of heat to or from the surroundings. In reaction dynamics, the word has been used in a microscopic sense, with a range of meanings which have only a tenuous relationship to the thermodynamic meaning or the etymology. Whereas the thermodynamic meaning relates to conditions imposed on a process by an observer, the microscopic meaning relates to conditions under which the process occurs naturally. The microscopic meanings, as used in reaction dynamics, all have in common the feature that quantum states remain unchanged during the course of reaction. Different quantum states may be referred to:

1. A reaction in which there is no change of electronic state or multiplicity has been called adiabatic, or more specifically electronically adiabatic.
2. A reaction in which there is no change of vibrational state during the course of reaction has been said to be vibrationally adiabatic. More loosely, the expression has been applied to a process in which excess vibrational energy in the reactants appears as vibrational energy in the products, or in which ground-state vibration in the reactants leads to ground state vibration in the products.
3. A reaction in which excess rotational energy in the reactants appears as rotational energy in the products, or in which ground-state rotation in the reactants leads to ground-state rotation in the products, has been referred to as rotationally adiabatic.
4. In the Rice-Ramsperger-Kassel-Marcus (RRKM) theory of unimolecular reactions, a degree of freedom whose quantum number is more or less preserved during energization and subsequent reaction has been called 'adiabatic'; the word 'inactive' has also been applied to it.

A reaction that is not adiabatic is referred to as nonadiabatic or diabatic, and some workers make a distinction between the two words.
See also: diabatic coupling

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 152

adiabatic electron transfer

Electron transfer process in which the reacting system remains on a single electronic surface in passing from reactants to products. For adiabatic electron transfer the electronic transmission factor is close to unity.
See: Marcus equation
See also: diabatic electron transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2227

adiabatic ionization

in mass spectrometry

A process whereby an electron is either removed from or added to an atom or molecule producing an ion in its ground state.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

adiabatic lapse rate

in atmospheric chemistry

The rate of decrease in temperature with increase in altitude of an air parcel which is expanding slowly to a lower atmospheric pressure without exchange of heat; for a descending parcel it is the rate of increase in temperature with decrease in altitude. Theory predicts that for dry air it is equal to the acceleration of gravity divided by the specific heat of dry air at constant pressure (approximately $9.8\ ^{\circ}\mathrm{C\ km^{-1}}$). The moist adiabatic lapse rate is less than the dry adiabatic lapse rate and depends on the moisture content of the air mass.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2171

adiabatic photoreaction

Within the 'Born-Oppenheimer' approximation, a reaction of an excited state species that occurs on a single 'potential-energy surface'.
See also: diabatic photoreaction

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2227

adiabatic transition-state theory

A form of transition-state theory in which the system is assumed to preserve its internal quantum states as it moves over the potential-energy surface. A detailed state-to-state scattering theory version of adiabatic transition-state theory has been referred to as the adiabatic channel model.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 152

adiabatic treatments of reaction rates

These are treatments of reaction rates in which the system is assumed to remain on a single potential-energy surface during the entire course of reaction, or to remain in a conserved internal state.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 152

adjacent re-entry model

in polymer crystals

A model of crystallinity in which chain folds regularly connect adjacent stems.

Source:
Purple Book, p. 84

adjuvant

1. In pharmacology, a substance added to a drug to speed or increase the action of the main component.
2. In immunology, a substance (such as aluminium hydroxide) or an organism (such as bovine tuberculosis bacillus) which increases the response to an antigen.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2010

adsorbate

A molecular species of gas, dissolved substance or liquid which adheres to or is adsorbed in an extremely thin surface layer of a solid substance.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2171
Orange Book, p. 85

adsorbent

A condensed phase at the surface of which adsorption may occur.

Source:
Orange Book, p. 85
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2171

adsorber

Solid material used to capture either a gas or liquid; often activated carbon is employed as the solid because of its high surface area per unit mass.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2171

adsorption

An increase in the concentration of a dissolved substance at the interface of a condensed and a liquid phase due to the operation of surface forces. Adsorption can also occur at the interface of a condensed and a gaseous phase.

Source:
Orange Book, p. 85
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2171

adsorption capacity

For strongly adsorbed solutes of limited solubility, the value of the amount of adsorbed substance reached in a saturated solution is called the adsorption capacity of the adsorbent for a specific solute; its value depends also, in general, on the nature and, in the case of more than two components, on the relative composition of the bulk liquid.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 594

adsorption chromatography

Chromatography in which separation is based mainly on differences between the adsorption affinities of the sample components for the surface of an active solid.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 826
Orange Book, p. 94

adsorption complex

The entity constituted by the adsorbate and the part of the adsorbent to which it is bound.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 74

See also:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 584

adsorption current

A faradaic current whose magnitude depends on the applied potential, and, at any particular applied potential, on the rate or extent of the adsorption of an electroactive substance (or the product obtained from the reduction or oxidation of an electroactive substance) onto the surface of the indicator or working electrode.
See also: limiting adsorption current

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1494

adsorption hysteresis

Adsorption hysteresis is said to occur when adsorption and desorption values deviate from one another.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 585

adsorption indicator

A substance which is adsorbed or desorbed with concomitant colour change at or near the equivalence point of a titration.

Source:
Orange Book, p. 48

adsorption isobar

The function relating the amount, mass, or volume, or corresponding excess of substance adsorbed by a given amount of solid, to the temperature at constant pressure.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 596

adsorption isostere

The function relating the equilibrium pressure to the temperature at a constant value of the amount, or excess amount, of substance adsorbed by a given amount of solid.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 596

adsorption isotherm

in chromatography

Isotherm describing adsorption of the sample component on the surface of the stationary phase from the mobile phase.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1592
This definition supersedes an earlier definition of adsorption isotherm.

adsorptive

The material that is present in one or other (or both) of the bulk phases and capable of being adsorbed.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 584

advancement

See: extent of reaction

Source:
Green Book, 2nd ed., p. 43

advection

in atmospheric chemistry

The transport of air, its properties (such as heat), trace materials, fog, cold air, etc., solely by mass motion of the atmosphere, generally in a horizontal direction.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2171

adverse effect

Change in biochemistry, morphology, physiology, growth, development, or lifespan of an organism which results in impairment of functional capacity or impairment of capacity to compensate for additional stress or increase in susceptibility to other environmental influences.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1038

aeration

in atmospheric chemistry

The process by which a volume filled with a liquid becomes permeated with air or another gas; aeration is often accomplished by spraying the liquid into the air, bubbling air through a liquid or agitating the liquid to promote surface absorption of air.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

aerobe

An organism that needs oxygen for respiration and hence for growth.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 145

aerobic

Requiring molecular oxygen.
See also: anaerobic

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2011

aerobic conditions

Conditions for growth or metabolism in which the organism is sufficiently supplied with oxygen.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 145

aerogel

Gel comprised of a microporous solid in which the dispersed phase is a gas.
Note:
Microporous silica, microporous glass and zeolites are common examples of aerogels.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1806

aeromete

in atmospheric chemistry

Instrument used to measure the density of gases.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

aerometric measurement

in atmospheric chemistry

A measurement of the temperature, pressure, air motion (velocity vectors), or other physical measurement to characterize an air mass.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

aerosol

Sol in which the dispersed phase is a solid, a liquid or a mixture of both and the continuous phase is a gas (usually air).
Notes:

1. Owing to their size, the particles of the dispersed phase have a comparatively small settling velocity and hence exhibit some degree of stability in the earth s gravitational field.
2. An aerosol can be characterized by its chemical composition, its radioactivity (if any), the particle size distribution, the electrical charge and the optical properties.
3. Modified from previous definition, within which particles with equivalent diameters usually between 0.01 and $100\ \mu\text{m}$ are specified. This extends beyond the size range specified for a *colloidal* system. To avoid confusion the definition proposed here is recommended.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1805

aerosol hydrolysis

Hydrolysis of the dispersed component of an aerosol.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1820

affine chain behaviour

Behaviour of a polymer network in which the junction points deform uniformly with the macroscopic deformation of the network.
Note:
In reality, affine chain behaviour can apply only at small deformations.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1818

affinity chromatography

An expression characterizing the particular variant of chromatography in which the unique biological specificity of the analyte and ligand interaction is utilized for the separation.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 826

See also:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 145

affinity of reaction, A

Negative partial derivative of Gibbs energy with respect to extent of reaction at constant pressure and temperature. It is positive for spontaneous reactions.
See also: driving force

Source:
Green Book, 2nd ed., p. 49

after mass analysis

in mass spectrometry

The sum of all the separate ion currents carried by the different ions contributing to the spectrum.

Source:
Orange Book, p. 206

ageing

of precipitate

The time-dependent change of those properties of a precipitate, e.g. loss of water, growth of crystals, recrystallization, decrease of the specific surface, loss of coprecipitated substances, which generally improve the filtering properties. The process of ageing is very often promoted by maintaining the precipitate and precipitation medium together at elevated temperatures for a period of time. The terms chemical, physical and thermal ageing may be used in cases in which some of the (usually combined) effects named above are to be emphasized specifically.

Source:
Orange Book, p. 86

agglomerate
Also contains definition of: aggregate *in polymer science*

in polymer science

Cluster of molecules or particles that results from agglomeration.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1803

agglomeration (except in polymer science)

Also contains definitions of: coagulation, flocculation

Process of contact and adhesion whereby dispersed particles are held together by weak physical interactions ultimately leading to phase separation by the formation of precipitates of larger than colloidal size.
Notes:
1. Agglomeration is a reversible process.
2. The definition proposed here is recommended for distinguishing agglomeration from aggregation.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1821

agglomeration
Also contains definition of: aggregation *in polymer science*

in polymer science

Process in which dispersed molecules or particles assemble rather than remain as isolated single molecules or particles.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1821

agglutination

An immunochemical reaction leading to the aggregation of particulate matter such as bacteria, erythrocytes or other cells, or synthetic particles such as plastic beads coated with antigens or antibodies.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 145

aggregate

Also contains definitions of: agglomerate *in catalysis*, primary particle *in catalysis*

in catalysis

Certain materials used as catalysts or supports consist of spheroids smaller than $10\ \mathrm{nm}$ in diameter, cemented into larger entities. A primary particle should be defined as the smallest discrete identifiable entity and the method of identification should be mentioned (e.g. transmission electron microscopy, scanning electron microscopy). An assemblage of such primary particles exhibiting an identifiable collective behaviour (e.g. chemical nature of the aggregated primary particles, texture of the aggregate, resistance to mechanical separation upon grinding) constitutes an aggregate. When describing the aggregates the criterion of identification should be mentioned. Strongly bonded aggregates are called agglomerates.

Source:
PAC, 1991, *63*, 1227 *(Manual on catalyst characterization (Recommendations 1991))* on page 1231

aggregation (except in polymer science)

Process whereby dispersed molecules or particles form aggregates.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1821

aging (ageing)

of a polymer

Processes that occur in a polymeric material during a specified period of time, and that usually result in changes in physical and/or chemical structure and the values of the properties of the material.

Source:
PAC, 1996, *68*, 2313 *(Definitions of terms relating to degradation, aging, and related chemical transformations of polymers (IUPAC Recommendations 1996))* on page 2315

aglycon (aglycone)

The non-sugar compound remaining after replacement of the glycosyl group from a glycoside by a hydrogen atom.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

agonist

Substance which binds to cell receptors normally responding to naturally occurring substances and which produces a response of its own.
See also: antagonist

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2011

agostic

The term designates structures in which a hydrogen atom is bonded to both a carbon atom and a metal atom. The term is also used to characterize the interaction between a CH bond and an unsaturated metal centre, and to describe similar bonding of a transition metal with Si–H compounds. The expression 'μ-hydrido-bridged' is also used to describe the bridging hydrogen.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1082

agostic interaction

The manner of interaction (termed according to the Greek 'to hold or clasp to oneself as a shield') of a coordinatively unsaturated metal atom with a ligand, when the metal atom draws the ligand towards itself. An important type of agostic interaction is the C–H–Metal coordination providing for the activation of the C–H bond in transition metal complexes.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1922

agranular carbon

A monogranular or monolithic carbon material with homogeneous microstructure which does not exhibit any structural components distinguishable by optical microscopy.
Note:
The above definition of a homogeneous microstructure does not pertain to pores and structural components which may be visible by contrast differences in optical microscopy with polarized light. As a consequence, glass-like carbon with visible pores is still an agranular carbon. The same is true, for instance, for pyrolytic carbon with preferred orientation, such as conical or lamellar structures, visible in optical microscopy with polarized light. Use of the term agranular carbon is not restricted to bulk materials of a minimum size. Only particulate carbon should be excluded even if the isolated particles exhibit a homogeneous microstructure.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 476

air contaminant

in atmospheric chemistry

A substance, gaseous material or aerosol, which is present in an air mass at levels greater than in clean air. An air contaminant has been added commonly by anthropogenic activity.
See also: air pollutant

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2182

air mass

in atmospheric chemistry

A qualitative term to describe a widespread body of air with approximately uniform characteristics which had been identified at a given time over a particular region of the earth's surface. Sometimes an air mass is marked by inert tracers such as SF_6 which may be added to it. The composition of a given air mass undergoes alteration as it migrates, chemical changes occur, compounds are removed by dry and wet deposition and new impurities are added to the mass.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

air monitoring station

in atmospheric chemistry

A site at which monitoring of the concentration of one or more pollutants is carried out (e.g. the BAPMoN stations, Background Air Pollution Monitoring Network of the WMO, World Meteorological Organization).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

air pollutant

A substance, gaseous material or aerosol which has been introduced into the air (either by human activity or by natural processes) in sufficient concentration to produce a measurable effect on humans, animals, vegetation or materials (monuments, etc.): SO_2, NO_2, H_2S, CO, hydrocarbons, etc.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

air pollution

Usually the presence of substances in the atmosphere, resulting either from human activity or natural processes, present in sufficient concentration, for a sufficient time and under circumstances such as to interfere with comfort, health or welfare of persons or the environment.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

air pollution index (air quality index)

A mathematical combination of the concentrations of air pollutants (weighted in some fashion to reflect the estimated health impact of the specific pollutant) which gives an approximate numerical measure of the quality of the air at a given time. These indices have little scientific basis but have been used to inform the public (in a qualitative fashion) of the degree of pollution present at a given time. It is recommended that the actual measured pollutant concentrations be used by all information services when possible with simultaneous reference given to the corresponding concentrations which are considered by health authorities to be hazardous to human health.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

air pollution survey

in atmospheric chemistry

A study of the concentrations and geographical distribution of specified air pollutants in a given area and an assessment of the damage, if any, which the pollutants have caused.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

air quality characteristic

in atmospheric chemistry

One of the quantifiable properties relating to an air sample: concentration of a constituent, wind speed, temperature, etc. The quantity of air quality characteristic is the true value of the characteristic being investigated; it is recognized that in practice, this value can only be approximated by existing methods.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

air resource management

in atmospheric chemistry

The detailed planning and the implementation of air pollution control programs designed to preserve the health and welfare of the people in the region, the plant and animal life, physical property, good visibility and other factors which determine the air quality and the maintenance of an aesthetically acceptable environment.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

air sampling network

in atmospheric chemistry

A number of air sampling stations which are established in a given geographical region at which measurements of both pollutant concentrations and meteorological quantities (wind speed, direction, rain fall, humidity, etc.) are made to determine the extent and the nature of the air pollution and to establish trends in the concentrations of the air pollutants with time.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

air-lift bioreactor

A bioreactor in which the reaction medium is kept mixed and gassed by introduction of air or another gas (mixture) at the base of a column-like reactor equipped either with a draught tube or another device (e.g. external tube) by which the reactor volume is separated into a gassed and an ungassed region thus generating a vertically circulating flow.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 146

Aitken particles

Aerosol particles below $0.1\ \mu m$ in diameter. These generally are the most numerous among all particles in the air. Their concentrations can be determined with the Aitken counter which measures total particle number density. Owing to their small size, Aitken particles contribute little to the total mass concentration of all aerosol particles; this is determined primarily by particles of diameter $> 0.1\ \mu m$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

albedo

The fraction of the energy of electromagnetic radiation reflected from a body (or surface) relative to the energy incident upon it. The reflection of light from a surface is, of course, dependent on the wavelength of the light, the nature of the surface and its angle of incidence with the surface. The term albedo usually connotes a broad wavelength band (visible, ultraviolet or infrared), whereas the terms reflectivity and spectral albedo are used to describe the reflection of monochromatic (single wavelength or small band of wavelengths) radiation.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

albumin

A type of protein, especially a protein of blood plasma which transports various substances, including metal ions, drugs and xenobiotics.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1255

alcogel

Gel in which the swelling agent consists predominantly of an alcohol or a mixture of alcohols.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1807

alcoholates

Synonymous with alkoxides. Alcoholate should not be used for solvates derived from an alcohol such as $CaCl_2 \cdot n ROH$, for the ending -ate often occurs in names for anions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

alcohols

Compounds in which a hydroxy group, –OH, is attached to a saturated carbon atom R_3COH. The term 'hydroxyl' refers to the radical species, $HO^{\cdot}$.
See also: enols, phenols

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

See also:
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

aldaric acids

Polyhydroxy dicarboxylic acids having the general formula $HOC(=O)[CH(OH)]_nC(=O)OH$, formally derived from an aldose by oxidation of both terminal carbon atoms to carboxyl groups.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312
White Book, p. 142

aldazines

Azines of aldehydes $RCH=NN=CHR$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

aldehydes

Compounds $RC(=O)H$, in which a carbonyl group is bonded to one hydrogen atom and to one R group.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

aldimines

Imines derived from aldehydes $RCH=NR$. E.g. $EtCH=NH$, $PhCH=NMe$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

alditols

Acyclic polyols having the general formula $HOCH_2[CH(OH)]_nCH_2OH$ (formally derivable from an aldose by reduction of the carbonyl group).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

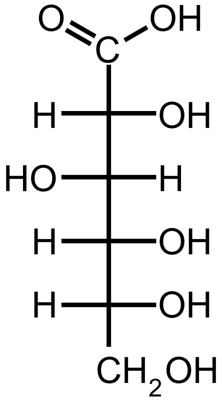
aldoketoses

A now less preferred synonym for ketoaldoses.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

aldonic acids

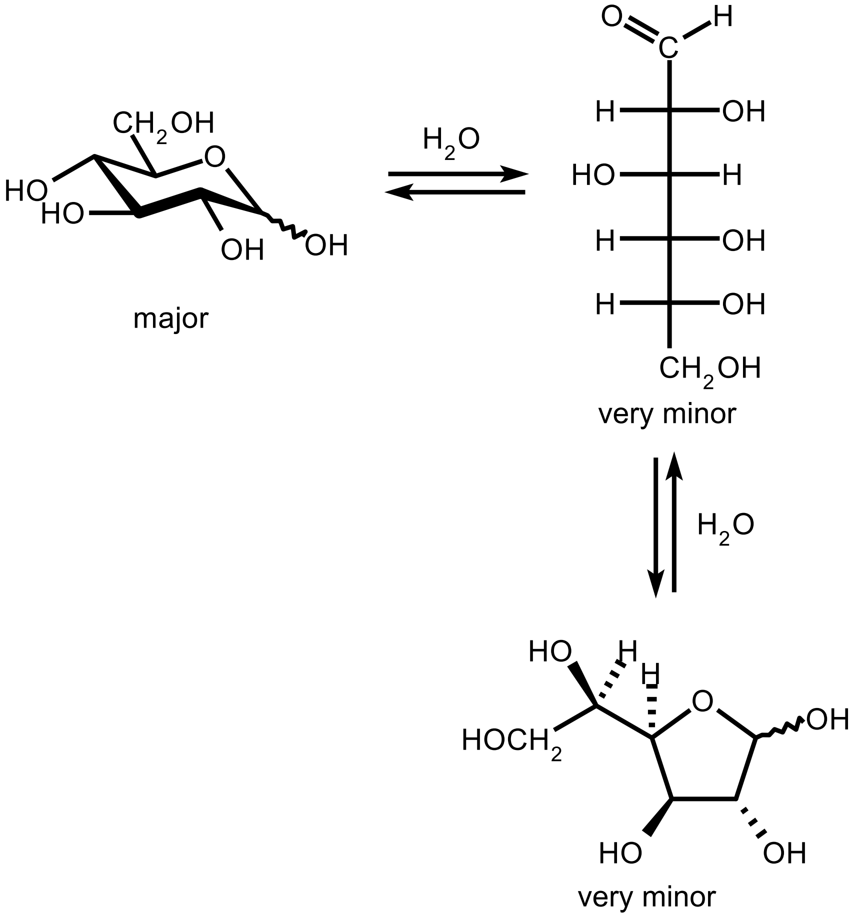
Polyhydroxy acids having the general formula $HOCH_2[CH(OH)]_nC(=O)OH$ and therefore derived from an aldose by oxidation of the aldehyde function, e.g. D-gluconic acid.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

aldoses

Aldehydic parent sugars (polyhydroxyaldehydes $H[CH(OH)]_nC(=O)H$, $n \geq 2$) and their intramolecular hemiacetals.



See also: monosaccharides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

aldoximes

Oximes of aldehydes RCH=NOH .

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

alert levels

in atmospheric chemistry

Designated concentrations of certain key pollutants at which some degree of danger to public health is expected. In many areas in which a relatively high level of pollution is often encountered, several levels of alert are often established. For example, a first alert may signify a potential problem exists; a second alert becomes a signal for the curtailment of certain significant emission sources; the third alert signifies the need for some specified emergency action which must be taken to ensure the public safety.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

alicyclic compounds

Aliphatic compounds having a carbocyclic ring structure which may be saturated or unsaturated, but may not be a benzenoid or other aromatic system.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

aliphatic compounds

Acyclic or cyclic, saturated or unsaturated carbon compounds, excluding aromatic compounds.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

aliquot

in analytical chemistry

A known amount of a homogeneous material, assumed to be taken with negligible sampling error. The term is usually applied to fluids. The term 'aliquot' is usually used when the fractional part is an exact divisor of the whole; the term 'aliquant' has been used when the fractional part is not an exact divisor of the whole (e.g. a $15\ \mathrm{ml}$ portion is an aliquant of $100\ \mathrm{ml}$). When a laboratory sample or test sample is 'aliquoted' or otherwise subdivided, the portions have been called split samples.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1206
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

alkaloids

Basic nitrogen compounds (mostly heterocyclic) occurring mostly in the plant kingdom (but not excluding those of animal origin). Amino acids, peptides, proteins, nucleotides, nucleic acids, amino sugars and antibiotics are not normally regarded as alkaloids. By extension, certain neutral compounds biogenetically related to basic alkaloids are included.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

alkalosis

Pathological condition in which the hydrogen ion substance concentration of body fluids is below normal and hence the pH of blood rises above the reference interval.
See also: acidosis

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2012

alkanes

Acyclic branched or unbranched hydrocarbons having the general formula C_nH_{2n+2} , and therefore consisting entirely of hydrogen atoms and saturated carbon atoms.
See also: cycloalkanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

alkanium ions

Carbocations derived from alkanes by *C*-hydronation containing at least one pentacoordinate carbon atom, E.g. $^{+}CH_5$ methanium, $[C_2H_7]^+$ ethanium.
See also: carbonium ions

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

alkene photocycloaddition

Photochemical process leading to formation of a cyclobutane upon addition of an electronically excited alkene to another ground-state alkene or of an electronically excited α,β-unsaturated carbonyl compound to a ground-state alkene. The latter is called a *de Mayo reaction*.
Note:
A special case of photocycloaddition is a photodimerization.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 301

alkene photodimerization

Photochemical process leading to the formation of a cyclobutane from two identical alkenes, i.e., from the photocycloaddition of an electronically excited alkene to a ground-state alkene.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 301

alkene photoisomerization

Photochemical process with geometrical isomerization of a carbon–carbon double bond.
Notes:

1. Geometrical isomerization of a C–C double bond is called a *cis/trans isomerization* in 1,2-disubstituted alkenes. *E*/*Z* isomerization is a more general designation applying also to higher substituted alkenes.
2. This process leads to a photostationary state if both isomers absorb light under the reaction conditions.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 302

alkene photorearrangement

Photochemical process leading to the skeletal rearrangement of an alkene.
See also: aza-di-π-methane rearrangement, di-π-methane rearrangement, di-π-silane rearrangement, oxa-di-π-methane rearrangement

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 302

alkenes

Acyclic branched or unbranched hydrocarbons having one carbon–carbon double bond and the general formula C_nH_{2n} . Acyclic branched or unbranched hydrocarbons having more than one double bond are alkadienes, alkatrienes, etc.
See also: olefins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1313

alkoxides

Compounds, ROM, derivatives of alcohols, ROH, in which R is saturated at the site of its attachment to oxygen and M is a metal or other cationic species.
See: alcoholates

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkoxyamines

O-Alkyl hydroxylamines (with or without substitution on N) $R'ONR_2$ ($R' \neq H$).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkyl groups

Univalent groups derived from alkanes by removal of a hydrogen atom from any carbon atom – C_nH_{2n+1}. The groups derived by removal of a hydrogen atom from a terminal carbon atom of unbranched alkanes form a subclass of normal alkyl (*n*-alkyl) groups $H(CH_2)_n$. The groups RCH_2, R_2CH ($R \neq H$), and R_3C ($R \neq H$) are primary, secondary and tertiary alkyl groups, respectively.
See also: cycloalkyl groups, hydrocarbyl groups

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkyl radicals

Carbon-centered radicals derived formally by removal of one hydrogen atom from an alkane, e.g. $CH_3CH_2C^{\cdot}H_2$ propyl.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkylenes

1. An old term, which is not recommended, for alkenes, especially those of low molecular weight.
2. An old term for alkanediyl groups commonly but not necessarily having the free valencies on adjacent carbon atoms, e.g. $–CH(CH_3)CH_2–$ propylene (systematically called propane-1,2-diyl).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkylidene groups

The divalent groups formed from alkanes by removal of two hydrogen atoms from the same carbon atom, the free valencies of which are part of a double bond, e.g. $(CH_3)_2C=$ propan-2-ylidene.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkylideneaminoxyl radicals

Radicals having the structure $R_2C{=}N{-}O^{\cdot}$. Synonymous with iminoxyl radicals.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkylideneaminyl radicals

Radicals having the structure $R_2C{=}N^{\cdot}$. Synonymous with iminyl radicals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkylidenes

Carbenes R_2C: formed by mono or dialkyl substitution of methylene, H_2C:, e.g. CH_3CH_2CH: propylidene.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkylidynes

Carbenes $R_2C^{\cdot\cdot\cdot}$ containing a univalent carbon atom, atom, e.g. $CH_3CH_2C^{\cdot\cdot\cdot}$ propylidyne

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

alkynes

Acyclic branched or unbranched hydrocarbons having a carbon-carbon triple bond and the general formula C_nH_{2n-2}, $RC{\equiv}CR$. Acyclic branched or unbranched hydrocarbons having more than one triple bond are known as alkadiynes, alkatriynes, etc.
See also: acetylenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

allele

One of several alternate forms of a gene which occur at the same locus on homologous chromosomes and which become separated during meiosis and can be recombined following fusion of gametes.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 146

allenes

Hydrocarbons (and by extension, derivatives formed by substitution) having two double bonds from one carbon atom to two others $R_2C{=}C{=}CR_2$. (The simplest member, propadiene, is known as allene).
See also: cumulenes, dienes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1314

allo-
in amino-acid nomenclature

Amino acids with two chiral centres were named in the past by allotting a name to the first diastereoisomer to be discovered. The second diastereoisomer, when found or synthesized, was then assigned the same name but with the prefix allo-. This method can be used only with trivial names but not with semisystematic or systematic names. It is now recommended that allo should be used only for alloisoleucine and allothreonine.

Source:
White Book, p. 46

allometric

Pertaining to a systematic relationship between growth rates of different parts of an organism and its overall growth rate.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1038

allosteric enzymes

Enzymes which contain regions to which small, regulatory molecules (cf. effector) may bind in addition to and separate from substrate binding sites. On binding the effector, the catalytic activity of the enzyme towards the substrate may be enhanced, in which case the effector is an activator, or reduced, in which case it is an inhibitor.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 146

allostery

A phenomenon whereby the conformation of an enzyme or other protein is altered by combination, at a site other than the substrate-binding site, with a small molecule, referred to as an effector, which results in either increased or decreased activity by the enzyme.

Source:
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

allotropes

Different structural modifications of an element.

Source:
Red Book, p. 35

allotropic transition

Synonym: allotriomorphic transition

A transition of a pure element, at a defined temperature and pressure, from one crystal structure to another which contains the same atoms but which has different properties. Examples: The transition of graphite to diamond, that of body-centred-cubic iron to face-centred-cubic iron, and the transition of orthorhombic sulfur to monoclinic sulfur. Synonymous with allotriomorphic transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 579

allylic groups

The group CH_2=$CHCH_2$ (allyl) and derivatives formed by substitution. The term 'allylic position' or 'allylic site' refers to the saturated carbon atom. A group, such as –OH, attached at an allylic site is sometimes described as 'allylic'.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1315

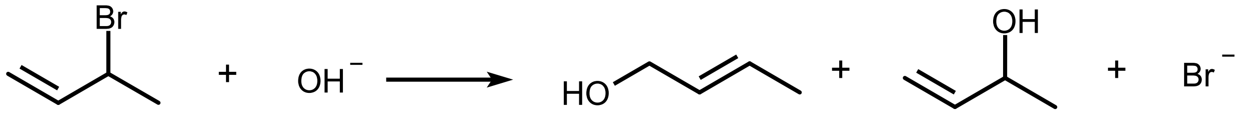
allylic intermediates

Carbanions, carbenium ions or radicals, formally derived by detachment of one hydron, hydride or hydrogen from the CH_3 group of propene or derivatives thereof. E.g. $H_2C{=}CHCH_2^+$ allyl cation.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1315

allylic substitution reaction

A substitution reaction occurring at position 1/ of an allylic system, the double bond being between positions 2/ and 3/. The incoming group may be attached to the same atom 1/ as the leaving group, or the incoming group becomes attached at the relative position 3/, with movement of the double bond from 2/3 to 1/2. For example:



(written as a transformation).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1082

alternancy symmetry

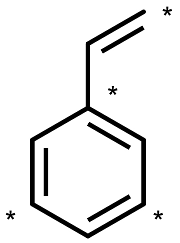
A topological property of the molecular graphs of alternant hydrocarbons which allows the carbon atoms to be divided into two subsets in such a way that no two atoms of the same subset are adjacent. A consequence of this property is the symmetrical arrangement of the energy levels of bonding and antibonding Hückel MOs relative to the level of a nonbonding orbital (energy level of the p AO of a carbon atom).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1922

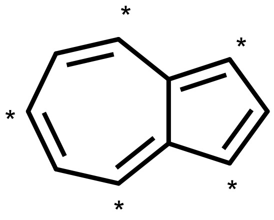
alternant

A conjugated system of π-electrons is termed alternant if its atoms can be divided into two sets so that no atom of one set is directly linked to any other atom of the same set.

Example of alternant π system:



Example of non-alternant π system:



(two atoms of unstarred set are directly linked)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1082

alternating copolymer

A copolymer consisting of macromolecules comprising two species of monomeric units in alternating sequence.
Note:
An alternating copolymer may be considered as a homopolymer derived from an implicit or hypothetical monomer.
See also: homopolymer (1)

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2301

alternating copolymerization

A copolymerization in which an alternating copolymer is formed.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2307

alternating current

Current with sinusoidal wave forms; all other wave forms should be termed 'periodic'.
See also: amplitude of alternating current

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1494

alternating voltage

This term should be applied only to sinusoidal phenomena; the term periodic voltage should be used for other wave forms.
See also: amplitude of alternating voltage

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1505

altocumulus cloud

in atmospheric chemistry

A dappled layer of patch or cloud composed of flattened globules that may be arranged in groups, lines or waves collectively known as billows; $2000 - 6000\ \mathrm{m}$; vertical velocities of $0.05\ - 0.1\ \mathrm{m\ s^{-1}}$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

altostratus cloud

in atmospheric chemistry

A grey, uniform, striated or fibrous sheet but without halo phenomena, and through which the sun is seen only as a diffuse, bright patch or not at all; usually at elevations $2000\ \mathrm{m} - 6000\ \mathrm{m}$; vertical velocities of $0.05\ \mathrm{m\ s^{-1}} - 0.1\ \mathrm{m\ s^{-1}}$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

AM 0 sunlight

Solar irradiance in space just above the atmosphere of the earth on a plane perpendicular to the direction of the sun (air mass, AM, zero). Also called extraterrestrial irradiance.
See also: AM 1 sunlight

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 302

AM 1 sunlight

Solar irradiance at sea level, i.e., traversing the atmosphere, when the direction of the sun is perpendicular to the surface of the earth. Also called terrestrial global irradiance.
See also: AM 0 sunlight

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 302

amalgam lamp

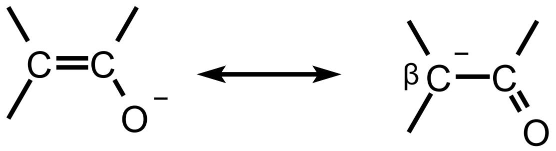
Intense source of *ultraviolet* (185 and 253.7 nm) radiation produced by an electrical discharge in a lamp with the inner side covered by an amalgam of mercury with another element such as indium or gallium to control the vapour pressure of the mercury. These lamps have 2-3 times the UV output for the same wavelength as the standard low-pressure mercury lamp.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 302

ambident

Also contains definitions of: multident, polydent

A description applied to a chemical species whose molecular entities each possess two alternative and strongly interacting distinguishable reactive centres, to either of which a bond may be made in a reaction: the centres must be connected in such a way that reaction at either site stops or greatly retards subsequent attack at the second site. The term is most commonly applied to conjugated nucleophiles, for example the enolate ion:



(which may react with electrophiles either at the β-carbon atom or at oxygen) or γ-pyridones, and also to the vicinally ambident cyanide ion, cyanate ion, thiocyanate ion, sulfinate ion, nitrite ion and unsymmetrical hydrazines. Ambident electrophiles are exemplified by carboxylic esters $RC(=O)OCR_3$ which react with nucleophiles either at the carbonyl carbon or the alkoxy carbon. Molecular entities, such as dianions of dicarboxylic acids, containing two non-interacting (or feebly interacting) reactive centres, are not generally considered to be ambident and are better described as 'bifunctional'. The Latin root of the word implies two reactive centres, but the term has in the past also incorrectly been applied to chemical species with more than two reactive centres. For such species the existing term 'polydent' (or, better, 'multident') is more appropriate.
See also: chelation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1082

ambient air

in atmospheric chemistry

The outdoor air in the particular location.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

ambient air quality

in atmospheric chemistry

A general term used to describe the quality of the outside air. Usually adjectives such as good, fair, bad, etc. are used by the media to describe this; often some form of air pollution or air quality index is employed to determine the specific descriptive term to be used. These are very qualitative terms of little or no scientific value.
See also: air pollution index

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

ambo

A prefix used to indicate that a molecule with two (or more) chiral elements is present as a mixture of the two racemic diastereoisomers in unspecified proportions. For example, the dipeptide formed from L-alanine and DL-leucine is L-alanyl-*ambo*-leucine.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2198

See also:
PAC, 1984, *56*, 595 *(Nomenclature and symbolism for amino acids and peptides (Recommendations 1983))* on page 595
PAC, 1982, *54*, 1507 *(Nomenclature of tocopherols and related compounds)* on page 1507

Ames/salmonella test

A screening test employed in predicting the mutagenic and the potential carcinogenic activities of chemicals in the environment. It employs Ames test strains of salmonella bacteria (his$^-$) which lack the ability to produce histidine. The compound to be tested, the bacteria and a small amount of histidine (insufficient to permit colony growth but enough to allow sufficient growth for expression of mutations) are added to agar. The bacteria are allowed to incubate for about $63\ \mathrm{h}$ at $37\ °\mathrm{C}$. If a significant increase in colonies above background is observed in the sample containing the test compound, then it is concluded that the chemical tested is a direct mutagen for the particular Ames strain of bacteria. This is taken as a qualitative indication of the possible carcinogenic activity of this chemical in other biological systems. This procedure seems to be of qualitative value in a preliminary screening of potential carcinogens.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2173

amic acids

Carbamoyl carboxylic acids, i.e. compounds containing a carboxy and a carboxamide group, e.g. 5-carbamoylnicotinic acid.
Note:
In systematic nomenclature replacement of the '-ic' suffix of a dicarboxylic acid by '-amic' is limited to dicarboxylic acids that have a trivial name. e.g. $HOC(=O)CH_2C(=O)NH_2$ malonamic acid (2-carbamoylacetic acid).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1315

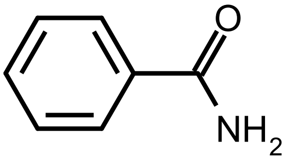
amide oximes

Compounds having the structure $RC(NH_2)=NOH$ and derivatives formed by substitution; formally the oximes of carboxamides

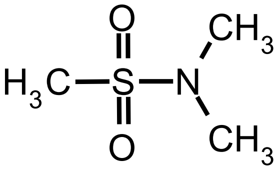
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1315

amides

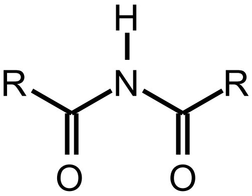
1. Derivatives of oxoacids $R_kE(=O)_l(OH)_m$ ($l \neq 0$) in which an acidic hydroxy group has been replaced by an amino or substituted amino group. Chalcogen replacement analogues are called thio-, seleno- and telluro-amides. Compounds having one, two or three acyl groups on a given nitrogen are generically included and may be designated as primary, secondary and tertiary amides, respectively, e.g.



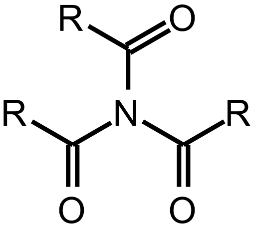
benzamide,



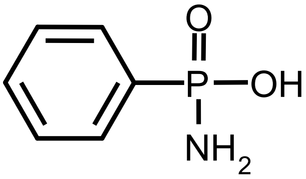
N,*N*-dimethylmethanesulfonamide,



secondary amides (see imides),



tertiary amides,

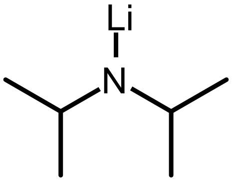


phenylphosphonamidic acid.

Notes:

1. Amides with NH_2, NHR and NR_2 groups should not be distinguished by means of the terms primary, secondary and tertiary.
2. Derivatives of certain acidic compounds $R_nE(OH)_m$, where E is not carbon (e.g. sulfenic acids, RSOH, phosphinous acids, R_2POH) having the structure $R_nE(NR_2)_m$ may be named as amides but do not belong to the class amides proper, e.g. $CH_3CH_2SNH_2$ ethanesulfenamide or ethylsulfanylamine.

2. The term applies also to metal derivatives of ammonia and amines, in which a cation replaces a hydrogen atom on nitrogen. Such compounds are also called azanides, e.g.



lithium diisopropylamide, synonym lithium diisopropylazanide.

See also: carboxamides, lactams, peptides, phosphoramides, sulfonamides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1315

See also:
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

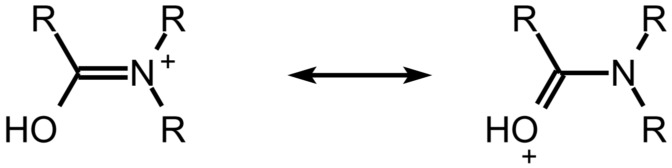
amidines

Derivatives of oxoacids $R_nE(=O)OH$ in which the hydroxy group is replaced by an amino group and the oxo group is replaced by =NR . Amidines include carboxamidines, sulfinamidines and phosphinamidines, $R_2P(=NR)NR_2$. In organic chemistry an unspecified amidine is commonly a carboxamidine.
See also: carboxamidines, sulfinamidines

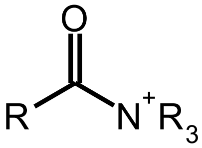
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1315

amidium ions

Cations formally derived by the addition of one hydron to the N or O atom of an amide and *N*-hydrocarbyl derivatives thereof. In organic chemistry an unspecified amidium ion is commonly a carboxamidium ion



or



The term does not imply knowledge concerning the position of the cationic centre, e.g. $PhC(=O)N^+Me_3$ *N,N,N*-trimethylbenzamidium.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1315

See also:
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

amidrazones

Also contains definitions of: amide hydrazones, hydrazide imides

Compounds having the structure $RC(=NH)NHNH_2$ or $RC(NH_2)=NNH_2$, formally derived from carboxylic acids. These tautomers are named hydrazide imides and amide hydrazones, respectively. Also included are *N*-hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

aminals

Compounds having two amino groups bonded to the same carbon, $R_2C(NR_2)_2$. Also called geminal diamines. [The term aminal has also been used, with consequent ambiguity, for α-amino ethers (hemiaminal ethers); such use is discouraged.]
See also: hemiaminals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

amine imides

Compounds formally derived from the attachment of an amine R_3N to a nitrene RN:. The structure $R_3N^+–N^-R$ expresses the 1,2-dipolar character of amine imides. They may be named systematically as substituted diazan-2-ium-1-ides, e.g. $Me_3N^+–N^-Me$, 1,2,2,2-tetramethyldiazan-2-ium-1-ide or trimethylamine *N*-methylimide.
See also: ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

See also:
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

amine imines [obsolete]

An undesirable synonym for amine imides
See: imides (2), ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

amine oxides

Compounds derived from tertiary amines by the attachment of one oxygen atom to the nitrogen atom $R_3N^+–O^-$. By extension the term includes the analogous derivatives of primary and secondary amines.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

amine ylides

Synonymous with ammonium ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

amines

Compounds formally derived from ammonia by replacing one, two or three hydrogen atoms by hydrocarbyl groups, and having the general structures RNH_2 (primary amines), R_2NH (secondary amines), R_3N (tertiary amines).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

aminimides **[obsolete]**

An undesirable synonym for amine imides.
See: ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

aminium ions

Cations HR_3N^+ formed by hydronation of an amine R_3N . 'Non-quaternary ammonium ions' is a synonymous term, e.g. prolinium, PhN^+HMe_2 , *N,N*-dimethylanilinium.
Note:

If a class X can be hydronated to Xium ions the class Xium ions commonly includes the derivatives formed by the replacement of the added hydron with a hydrocarbyl group. Aminium ions form an exception, made possible by the availability of the class name ammonium ions.
See also: onium compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

aminiumyl radical ions

Radicals cations, $R_3N^{\cdot +}$ derivable from aminium ions, R_3NH^+ , by removal of a hydrogen atom. Aminiumyl radical ions are, except for $H_3N^{\cdot +}$, synonymous with the ammoniumyl radical ions. As the term ammonium is well known, ammoniumyl radical ions is the more desirable class name.
See: ammoniumyl radical ions

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

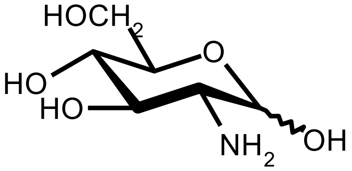
amino radicals [obsolete]

A non-IUPAC term for aminyl radicals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1316

amino sugars

Monosaccharides having one alcoholic hydroxy group (commonly but not necessarily in position 2) replaced by an amino group; systematically known as *x*-amino-*x*-deoxymonosaccharides. (Glycosylamines are excluded.)
E.g. D-glucosamine or 2-amino-2-deoxy-D-glucopyranose.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

amino-acid residue

Also contains definition of: N-terminal residue *in a polypeptide*

in a polypeptide

When two or more amino acids combine to form a peptide, the elements of water are removed, and what remains of each amino acid is called an amino-acid residue. α-Amino-acid residues are therefore structures that lack a hydrogen atom of the amino group (–NH–CHR–COOH), or the hydroxyl moiety of the carboxyl group (NH_2–CHR–CO–), or both (–NH–CHR–COO–); all units of a peptide chain are therefore amino-acid residues. (Residues of amino acids that contain two amino groups or two carboxyl groups may be joined by isopeptide bonds, and so may not have the formulas shown.) The residue in a peptide that has an amino group that is free, or at least not acylated by another amino-acid residue (it may, for example, be acylated or formylated), is called N-terminal; it is at the N-terminus. The residue that has a free carboxyl group, or at least does not acylate another amino-acid residue, (it may, for example, acylate ammonia to give –NH–CHR–CO–NH_2), is called C-terminal.

Source:
White Book, p. 48

aminonitrenes [obsolete]

An incorrect name for isodiazenes.
See: carbene analogues

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

aminooxyl radicals

See: aminoxyl radicals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

See also:
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

aminoxides

The anion $H_2N–O^-$, aminoxide and its N hydrocarbyl derivatives $R_2N–O^-$; formally derived from hydroxylamines, $R_2N–OH$, by removing a hydron from the hydroxy group, e.g. $(CH_3)_2N–O^-$ dimethylaminoxide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

See also:
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

aminoxyl radicals

Compounds having the structure $R_2N–O^{\cdot} \longleftrightarrow R_2N^{\cdot+}–O^{-}$; they are radicals derived from hydroxylamines by removal of the hydrogen atom from the hydroxy group, and are in many cases isolable. The synonymous terms 'nitroxyl radicals' and 'nitroxides' erroneously suggest the presence of a nitro group; their use is not desirable. E.g. $(ClCH_2)_2N–O^{\cdot}$ bis(chloromethyl)aminoxyl.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

See also:
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

aminyl oxides **[obsolete]**

Obsolete term for aminoxyl radicals.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

aminyl radicals

The nitrogen-centered radical $H_2N^{\cdot}$, formally derived by the removal of a hydrogen atom from ammonia, and its hydrocarbyl derivatives $R_2N^{\cdot}$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

ammonium compounds

See: onium compounds.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

ammonium imines **[obsolete]**

An undesirable synonym for amine imides

See: ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

ammonium ylides

1,2-Dipolar compounds of general structure $R_3N^+–C^-R_2$.
See also: ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

ammoniumyl radical ions

$H_3N^{\cdot+}$ and its hydrocarbyl derivatives, e.g. $(CH_3)_3N^{\cdot+}$ trimethylammoniumyl, $PhN^{\cdot+}H_2$ phenylammoniumyl or benzenaminiumyl.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

See also:
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

amorphous carbon

A carbon material without long-range crystalline order. Short-range order exists, but with deviations of the interatomic distances and/or interbonding angles with respect to the graphite lattice as well as to the diamond lattice.
Note:
The term amorphous carbon is restricted to the description of carbon materials with localized π-electrons as described by P.W.Anderson (*Phys. Rev.*, 1958, *109*, 1492). Deviations in the C–C distances greater than 5% (i.e. $\frac{\Delta x}{x_0} > 0.05$, where x_0 is the inter-atomic distance in the crystal lattice for the sp^2 as well as for the sp^3 configuration) occur in such materials, as well as deviations in the bond angles because of the presence of 'dangling bonds'. The above description of amorphous carbon is not applicable to carbon materials with two-dimensional structural elements present in all pyrolysis residues of carbon compounds as polyaromatic layers with a nearly ideal interatomic distance of $a = 142\ \mathrm{pm}$ and an extension greater than $1000\ \mathrm{pm}$.
See also: diamond-like carbon films

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 477

amount concentration, *c*

Amount of a constituent divided by the volume of the mixture. Also called amount-of-substance concentration, substance concentration (in clinical chemistry) and in older literature molarity. For entities B it is often denoted by $[\mathrm{B}]$. The common unit is mole per cubic decimetre ($\mathrm{mol\ dm^{-3}}$) or mole per litre ($\mathrm{mol\ L^{-1}}$) sometimes denoted by M.
See also: concentration

Source:
Green Book, 2nd ed., p. 42

amount fraction, *x* (*y* for gaseous mixtures)

Synonym: mole fraction

Amount of a constituent divided by the total amount of all constituents in the mixture. It is also called mole fraction. Amount fraction is equal to the number fraction: the number of entities of one constituent divided by the total number of entities in the mixture.
See also: fraction

Source:
Green Book, 2nd ed., p. 41

amount of substance, *n*

Also contains definition of: number of moles

Base quantity in the system of quantities upon which SI is based. It is the number of elementary entities divided by the Avogadro constant. Since it is proportional to the number of entities, the proportionality constant being the reciprocal Avogadro constant and the same for all substances, it has to be treated almost identically with the number of entities. Thus the counted elementary entities must always be specified. The words 'of substance' may be replaced by the specification of the entity, for example: amount of chlorine atoms, n_{Cl}, amount of chlorine molecules, $n(\mathrm{Cl_2})$. No specification of the entity might lead to ambiguities [amount of sulfur could stand for $n(\mathrm{S})$, $n(\mathrm{S_8})$, etc.], but in many cases the implied entity is assumed to be known: for molecular compounds it is usually the molecule [e.g. amount of benzene usually means $n(\mathrm{C_6H_6})$], for ionic compounds the simplest formula unit [e.g. amount of sodium chloride usually means $n(\mathrm{NaCl})$] and for metals the atom [e.g. amount of silver usually stands for $n(\mathrm{Ag})$]. In some derived quantities the words 'of substance' are also omitted, e.g. amount concentration, amount fraction. Thus in many cases the name of the base quantity is shortened to amount and to avoid possible confusion with the general meaning of the word the attribute chemical is added. The chemical amount is hence the alternative name for amount of substance. In the field of clinical chemistry the words 'of substance' should not be omitted and abbreviations such as substance concentration (for amount of substance concentration) and substance fraction are in use. The quantity had no name prior to 1969 and was simply referred to as the number of moles.

Source:
Green Book, 2nd ed., p. 46

PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 961

amount-of-substance concentration

Synonymous with amount concentration

Source:
Green Book, 2nd ed., p. 42

amount-of-substance fraction, x

Synonymous with amount fraction.

Source:
Green Book, 2nd ed., p. 41

ampere

SI base unit for the electric current (symbol: A). The ampere is that constant current which, if maintained in two straight parallel conductors of infinite length, of negligible circular cross-section, and placed 1 metre apart in vacuum, would produce between these conductors a force equal to 2×10^{-7} newton per metre of length (9th CGPM, 1948).

Source:
Green Book, 2nd ed., p. 70
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 961

amperometric detection method

in electrochemical analysis

A detection method in which the current is proportional to the concentration of the species generating the current.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

amphipathic

The property of surface activity is usually due to the fact that the molecules of the substance are amphipathic or amphiphilic, meaning that each contains both a hydrophilic and a hydrophobic (lipophilic) group. This assumes that one of the two phases is aqueous, and the other non-aqueous. If both are non-aqueous (e.g. oil/air), molecules containing organophilic and organophobic groups may be amphipathic and surface active.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

amphiphilic

A term used to describe a compound containing a large organic cation or anion which possesses a long unbranched hydrocarbon chain, e.g.

$CH_3(CH_2)_nCO_2^-M^+$

$CH_3(CH_2)_nN^+(CH_3)_3X^-$ ($n > 7$)

$CH_3(CH_2)_nSO_3^-M^+$.

The existence of distinct polar (hydrophilic) and nonpolar (hydrophobic) regions in the molecule promotes the formation of *micelles* in dilute aqueous solution.
See also: amphipathic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1083

amphiprotic (solvent)

Self-ionizing solvent possessing both characteristics of Brønsted acids and bases, for example H_2O and CH_3OH, in contrast to aprotic solvent.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1083
Orange Book, p. 30

ampholytes

See: zwitterionic compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

ampholytic polymer

Synonym: polyampholyte

Polyelectrolyte composed of macromolecules containing both cationic and anionic groups, or corresponding ionizable groups.
Note:
An ampholytic polymer in which ionic groups of opposite sign are incorporated into the same pendant groups is called, depending on the structure of the pendant groups, a zwitterionic polymer, polymeric inner salt, or polybetaine.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2068

amphoteric

A chemical species that behaves both as an acid and as a base is called amphoteric. This property depends upon the medium in which the species is investigated: H_2SO_4 is an acid when studied in water, but becomes amphoteric in superacids.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1083

amplification reaction

A reaction which replaces the conventional reaction used in a particular determination so that a more favourable measurement can be made. The sequence can be repeated to provide a further favourable increase in measurement.

Source:
PAC, 1982, *54*, 2553 *(Recommendations on use of the term amplification reactions)* on page 2554

amplitude of alternating current

Half the peak-to-peak amplitude of a sinusoidal alternating current.

Source:
Orange Book, p. 53
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1494

amplitude of alternating voltage

This term should denote half of the peak-to-peak amplitude. Peak-to-peak and r.m.s. amplitudes should be so specified.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1505

anabolism

The processes of metabolism that result in the synthesis of cellular components from precursors of low molecular weight.
See also: catabolism

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 146
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2013

anaerobe

An organism that does not need free-form oxygen for growth. Many anaerobes are even sensitive to free oxygen. Obligate (strict) anaerobes grow only in the absence of oxygen. Facultative anaerobes can grow either in the presence or in the absence of molecular oxygen.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 146

anaerobic

Not requiring molecular oxygen.
See also: aerobic

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2013

anaesthetic

Substance which produces loss of feeling or sensation: general anaesthetic produces loss of consciousness; local or regional anaesthetic renders a specific area insensible to pain.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2013

analgesic

Substance which relieves pain, without causing loss of consciousness.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2013

analogue metabolism

Process by which a normally non-biodegradable compound is biodegraded in the presence of a structurally similar compound which can induce the necessary enzymes.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2013

analogue to digital converter (pulse)

A pulse amplitude analyser which, for each pulse processed, produces an integer proportional to the height of that pulse.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

analyte

The component of a system to be analysed.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

analytical function

A function which relates the measured value $\hat{C}_\mathrm{a}$ to the instrument reading, X, with the value of all interferants, C_i, remaining constant. This function is expressed by the following regression of the calibration results.

$$\hat{C}_\mathrm{a} = f(X)$$

The analytical function is taken as equal to the inverse of the calibration function.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

analytical instrument

A device or a combination of devices used to carry out an analytical process. The analytical process is all or part of the analytical procedure that encompasses all steps from the introduction of the sample or the test portion to the production of the result. An analytical instrument may carry out single or multiple analytical procedures. In the latter case it may be selective, i.e. designed to carry out any requested combination of procedures within the set, on each specimen.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1659

analytical intercomparison

A procedure which gives insight to the accuracy of results of analytical procedures by comparing the results obtained in the analyses of identical samples at different laboratories and preferably with different analytical methods.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1544

analytical pyrolysis

The characterization, in an inert atmosphere, of a material or a chemical process by a chemical degradation reaction(s) induced by thermal energy.

Source:
PAC, 1993, *65*, 2405 *(Nomenclature and terminology for analytical pyrolysis (IUPAC Recommendations 1993))* on page 2406

analytical quality control

Procedures which give insight into the precision and accuracy of analysis results.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

analytical radiochemistry

Synonym: radioanalytical chemistry

That part of analytical chemistry in which the application of radioactivity is an essential step in the analytical procedures. Synonymous with radioanalytical chemistry.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

analytical sample

See: sample *in analytical chemistry*, test sample

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1200
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1206

analytical unit (analyser)

An assembly of subunits comprising: suitable apparatus permitting the introduction and removal of the gas, liquid or solid to be analysed and/or calibration materials; a measuring cell or other apparatus which, from the physical or chemical properties of the components of the material to be analysed, gives signals allowing their identification and/or measurement; signal processing devices (amplification, recording) or, if need be, data processing devices.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

anation

Replacement of the ligand water by an anion in a coordination entity.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1257

aneroid barometer

An instrument for monitoring the atmospheric pressure in which no liquid is employed, but rather changes in pressure between the atmosphere and a closed vessel bend a diaphram which moves a pointer on a scale.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

Anger camera

A camera in which a large diameter scintillator is coupled to an array of photomultiplier tubes by fibre optics. X-ray imaging may also be achieved in multi-crystal cameras where many small crystals individually scintillate.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1756

angle

The angle between two half-lines terminating at the same point is the ratio of the length of the included arc of the circle (with its centre at that point) to the radius of the circle. Symbols: α,β,γ ... This is a quantity of dimension one with the SI unit radian (rad), but very often degrees of arc are used.

Source:
Green Book, 2nd ed., p. 11

PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 961

angle of optical rotation, α

Angle through which plane polarized light is rotated clockwise, as seen when facing the light source, in passing through an optically active medium.

Source:
Green Book, 2nd ed., p. 33

angle strain

Synonym: Baeyer strain

Strain due to a departure in bond angle from 'normal' values. The term is often used in the context of non-aromatic cyclic compounds in which the internal angles differ from the regular tetrahedral angle of $109\ °\ 28'$; in this sense angle strain is also known as Baeyer strain.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2198

ångström

Non-SI unit of length, $\text{Å} = 10^{-10}\ \text{m}$, widely used in molecular physics.

Source:
Green Book, 2nd ed., p. 75
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 961

angular distribution

With reference to the center of mass, the products of a bimolecular reaction are scattered with respect to the initial velocity vector, and the distribution of scattering angles is known as the angular distribution.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 153

angular frequency, ω

Synonyms: circular frequency, pulsatance

Frequency multiplied by 2π. Also called pulsatance. It was formerly called circular frequency.

Source:
Green Book, 2nd ed., p. 11

angular momentum, *L*

Angular momentum, or moment of momentum of a particle about a point is a vector quantity equal to the vector product of the position vector of the particle and its momentum, $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$. For special angular momenta of particles in atomic and molecular physics different symbols are used.

Source:
Green Book, 2nd ed., p. 12

angular overlap model (AOM)

A method of description of transition metal–ligand interactions and main group stereochemistry, whose basic assumption is in that the strength of a bond formed using atomic orbitals on two atoms is related to the magnitude of overlap of the two orbitals.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1923

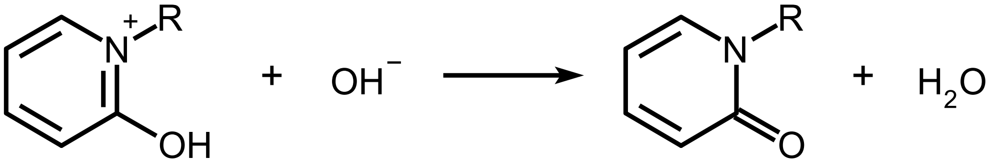
anhydrides

See: acid anhydrides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

anhydro bases

Compounds resulting from internal acid–base neutralization (with loss of water) in iminium hydroxides containing an acidic site conjugated with the iminium function.



See: pseudo bases

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

anilides

1. Compounds derived from oxoacids $R_kE(=O)_l(OH)_m$ ($l \neq 0$) by replacing an OH group by the NHPh group or derivative formed by ring substitution; *N*-phenyl amides, e.g. $CH_3C(=O)NHPh$ acetanilide.
   See: amides
2. Salts formed by replacement of a nitrogen-bound hydron of aniline by a metal or other cation, e.g. NaNHPh sodium anilide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

anils

A term for the subclass of Schiff bases $R_2C=NR'$, where R' = phenyl or substituted phenyl group. Thus, *N*-phenyl imines.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1317

anion

A monoatomic or polyatomic species having one or more elementary charges of the electron.

Source:
Red Book, p. 107

anion exchange

The process of exchanging anions between a solution and an anion exchanger.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 854

anion exchanger

Ion exchanger with anions as counter-ions. The term anion-exchange resin may be used in the case of solid organic polymers. The base form of an anion exchanger is the ionic form in which the counter-ions are hydroxide groups (OH– form) or the ionogenic groups form an uncharged base, e.g. –NH .

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 856

anion-exchange polymer

See also: ion-exchange polymer.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2069

anionic polymer

Polymer composed of negatively charged macromolecules and an equivalent amount of counter-cations.
Notes:

1. If a substantial fraction of constitutional units carries negative charges, then an anionic polymer is a polyelectrolyte.
2. The term anionic polymer should not be used to denote a polymer prepared by anionic polymerization.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2069

anionic polymerization

An ionic polymerization in which the kinetic-chain carriers are anions.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2308

anionotropic rearrangement (or anionotropy)

A rearrangement in which the migrating group moves with its electron pair from one atom to another.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1083

anisotropy

The property of molecules and materials to exhibit variations in physical properties along different molecular axes of the substance.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1257

annelation

Alternative, but less desirable term for annulation. The term is widely used in the German and French languages.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1083

annihilation

Also contains definition of: energy pooling

1. (*in radiochemistry*) An interaction between a particle and its antiparticle in which they both disappear.

   Source:
   Orange Book, p. 211
2. (*in photochemistry*) Two atoms or molecular entities both in an excited electronic state interact often (usually upon collision) to produce one atom or molecular entity in an excited electronic state and another in its ground electronic state. This phenomenon (annihilation) is sometimes referred to as energy pooling.
   See: singlet-singlet annihilation, spin-conservation rule, triplet-triplet annihilation

   Source:
   PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2228

annulation

A transformation involving fusion of a new ring to a molecule via two new bonds. Some authors use the term 'annelation' for the fusion of an additional ring to an already existing one, and 'annulation' for the formation of a ring from one or several acyclic precursors, but this distinction is not made generally.
See also: cyclization

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1083

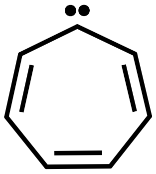
annulenes

Mancude monocyclic hydrocarbons without side chains of the general formula C_nH_n (n is an even number) or C_nH_{n+1} (n is an odd number). In systematic nomenclature an annulene with seven or more carbon atoms may be named [*n*]annulene, where n is the number of carbon atoms, e.g. [9]annulene for cyclonona-1,3,5,7-tetraene.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1083

annulenylidenes

Carbenes, derived by formal insertion of a divalent carbon atom into an even-membered annulene, e.g. cycloheptatrienylidene:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318

anode

Electrode at which oxidation takes place.

Source:
Green Book, 2nd ed., p. 59

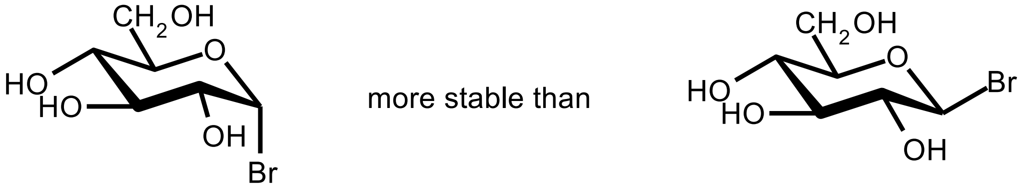
anodic transfer coefficient

Defined by analogy with cathodic transfer coefficient.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 515

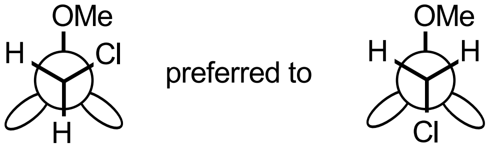
anomeric effect

Originally the thermodynamic preference for polar groups bonded to C-1 (the anomeric carbon of a glycopyranosyl derivative) to take up an axial position.

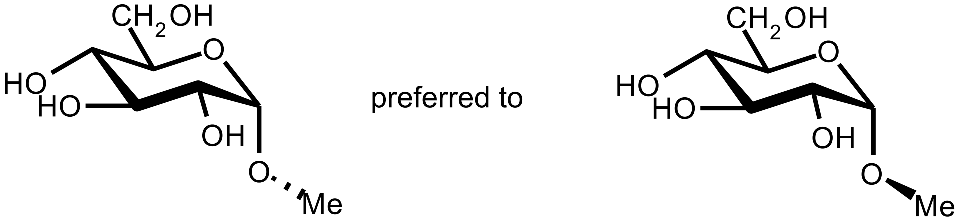


This effect is now considered to be a special case of a general preference (the generalized anomeric effect) for synclinal (gauche) conformations about the bond C–Y in the system X–C–Y–C where

X and Y are heteroatoms having nonbonding electron pairs, commonly at least one of which is nitrogen, oxygen or fluorine. For example in chloro(methoxy)methane the anomeric effect stabilizes the synclinal conformation.



In alkyl glycopyranosides the anomeric effect operates at two sites (i) along the endocyclic C-1 oxygen bond (endo-anomeric effect) and (ii) along the exocyclic C-1 oxygen bond (exo-anomeric effect). The opposite preference is claimed for some systems e.g. glycopyranosyltrialkylammonium salts, and has been referred to as the reverse anomeric effect.



Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2198

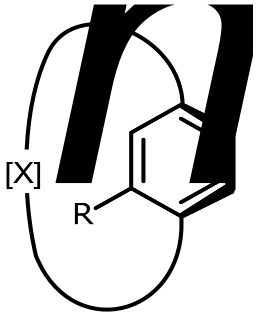
anomers

Diastereoisomers of glycosides, hemiacetals or related cyclic forms of sugars, or related molecules differing in configuration only at C-1 of an aldose, C-2 of a 2-ketose, etc.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2199

ansa compounds

Benzene derivatives having *para* positions (or *meta*) bridged by a chain (commonly 10 to 12 atoms long) (Latin *ansa*, handle). By extension, any arene bridged by a chain constrained to lie over one of the two faces of the arene.



See: cyclophanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318

antagonism

Combined effect of two or more factors which is smaller than the solitary effect of any one of those factors. In bioassays, the term may be used when a specified response is produced by exposure to either of two factors but not by exposure to both together.
See also: synergism

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2014

antagonist

1. Substance that reverses or reduces the effect induced by an agonist.
2. Substance that attaches to and blocks cell receptors that normally bind naturally occurring substances.

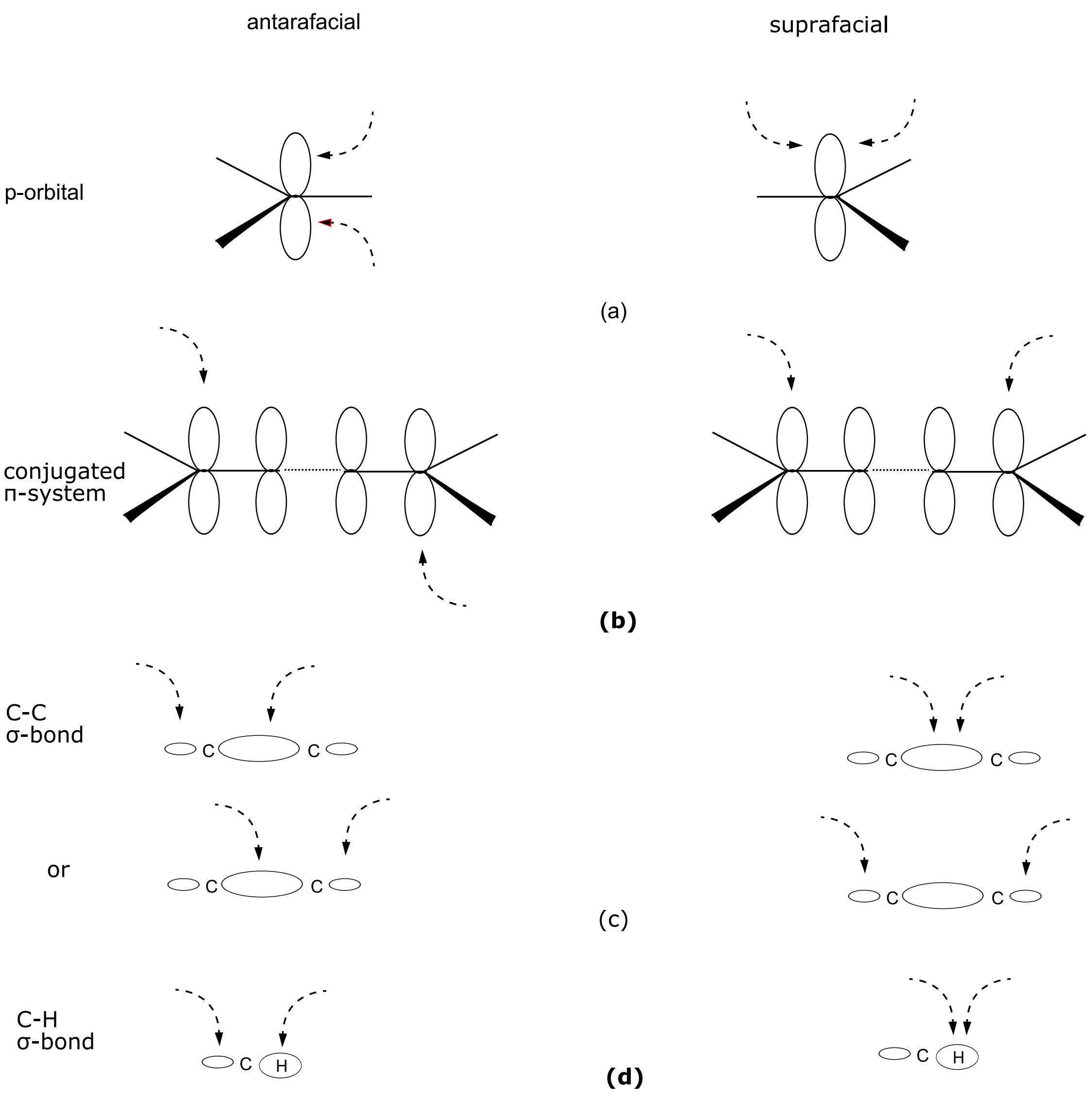
See also: agonist

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2014

antarafacial

Also contains definition of: suprafacial

When a part of a molecule ('molecular fragment') undergoes two changes in bonding (bond-making or bond-breaking), either to a common centre or to two related centres, external to itself, these bonding changes may be related in one of two spatially different ways. These are designated as 'antarafacial' if opposite faces of the molecular fragment are involved, and 'suprafacial' if both changes occur at the same face. The concept of 'face' is clear from the diagrams in the cases of planar (or approximately planar) frameworks with isolated or interacting p-orbitals [diagrams (a) and (b)].



The terms antarafacial and suprafacial are, however, also employed in cases in which the essential part of the molecular fragment undergoing changes in bonding comprises two atoms linked only by a σ-bond. In these cases it is customary to refer to the phases of the local σ-bonding orbital: occurrence of the two bonding changes at sites of like orbital phase is regarded as suprafacial, whereas that at two sites of opposite phase is antarafacial. The possibilities are shown for C–C and C–H σ-bonds in diagrams (c) and (d). There may be two distinct and alternative stereochemical outcomes of a suprafacial process involving a σ-bond between saturated carbon atoms, i.e. either retention or inversion at both centres. The antarafacial process results in inversion at one centre and retention at the second. For examples of the use of these terms, see cycloaddition, sigmatropic rearrangement.
See also: anti, sigma, pi

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1084

anthelmint(h)ic

Synonym: antihelminth

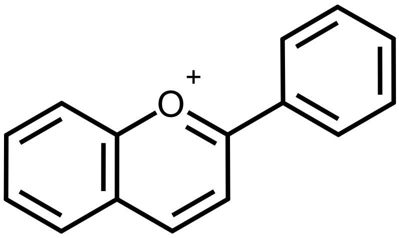
Substance intended to kill parasitic intestinal worms, such as helminths. Synonymous with antihelminth.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2014

anthocyanidins

Also contains definition of: flavylium salts

Aglycons of anthocyanins ; they are oxygenated derivatives of flavylium (2-phenylchromenylium) salts.



See: flavonoids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318

anthocyanins

Plant pigments of the flavonoid class; they are glycosides that on hydrolysis yield coloured aglycons called anthocyanidins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318

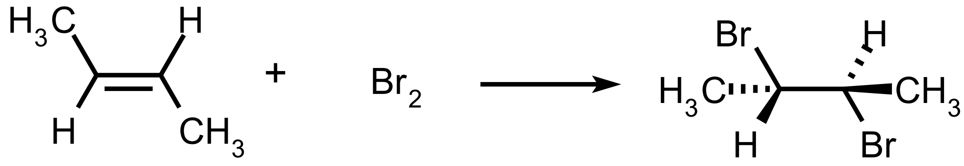
anti

In the representation of stereochemical relationships 'anti' means 'on opposite sides' of a reference plane, in contrast to 'syn' which means 'on the same side', as in the following examples.

1. Two substituents attached to atoms joined by a single bond are anti if the torsion angle (dihedral angle) between the bonds to the substituents is greater than 90°, or syn if it is less than 90°. (A further distinction is made between antiperiplanar, synperiplanar, anticlinal and synclinal.)

2. In the older literature the terms anti and syn were used to designate stereoisomers of oximes and related compounds. That usage was superseded by the terms 'trans' and 'cis' or *E* and *Z*, respectively.
3. When the terms are used in the context of chemical reactions or transformations, they designate the relative orientation of substituents in the substrate or product:
   1. Addition to a carbon-carbon double bond:

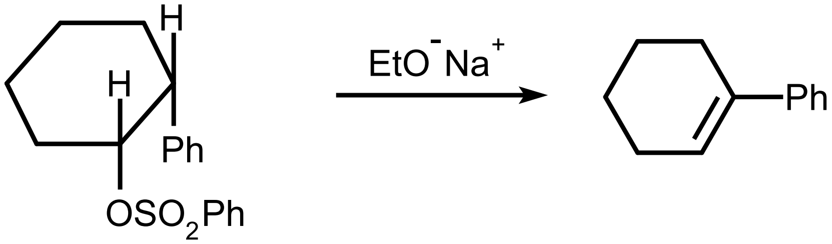
anti:



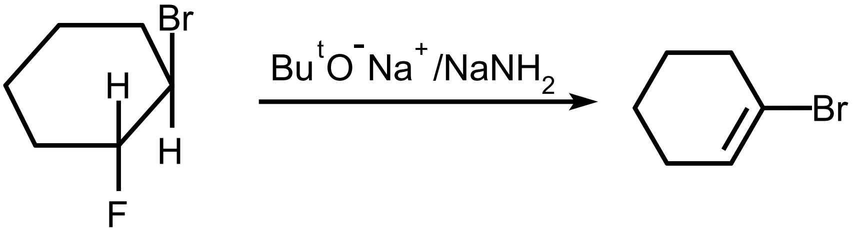
syn:

   2. Alkene-forming elimination:

anti:



syn:



In the examples described under (1) and (2) anti processes are always antarafacial, and syn processes are suprafacial.

See also: endo, exo, syn, anti

Source:

PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1084

PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2199

anti-Compton γ-ray spectrometer

A gamma-ray spectrometer in which the effect of the Compton scattering is at least partly compensated.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

anti-Hammond effect

See: More O'Ferrall-Jencks diagram.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1085

anti-Stokes type radiation (fluorescence)

Fluorescence radiation occurring at shorter wavelengths than absorption.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 236

anti-thixotropy

Opposite of thixotropy.
See also: work hardening

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

antiaromatic compounds

Compounds that contain $4n$ $(n \neq 0)$ π-electrons in a cyclic planar, or nearly planar, system of alternating single and double bonds, e.g. cyclobuta-1,3-diene.
See also: aromatic compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318

antiaromaticity (antithetical to aromaticity)

Those cyclic molecules for which cyclic electron delocalization provides for the reduction (in some cases, loss) of thermodynamic stability compared to acyclic structural analogues are classified as antiaromatic species. In contrast to aromatic compounds, antiaromatic ones are prone to reactions causing changes in their structural type, and display tendency to alternation of bond lengths and fluxional behavior (see fluxional molecules) both in solution and in the solid. Antiaromatic molecules possess negative (or very low positive) values of resonance energy and a small energy gap between their highest occupied and lowest unoccupied molecular orbitals. In antiaromatic molecules, an external magnetic field induces a paramagnetic electron current. Whereas benzene represents the prototypical aromatic compound, cyclobuta-1,3-diene exemplifies the compound with most clearly defined antiaromatic properties.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1923

antibiotic

Substance produced by, and obtained from, certain living cells (especially bacteria, yeasts and moulds), or an equivalent synthetic substance, which is biostatic or biocidal at low concentrations to some other form of life, especially pathogenic or noxious organisms.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2014

antibody

A protein (immunoglobulin) produced by the immune system of an organism in response to exposure to a foreign molecule (antigen) and characterized by its specific binding to a site of that molecule (antigenic determinant or epitope).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 146
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2014

antibonding molecular orbital

The molecular orbital whose occupation by electrons decreases the total bonding (as usual, increases the total energy) of a molecule. The energy level of an antibonding MO lies higher than the average of the valence atomic orbitals of the atoms constituting the molecule.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1923

anticholinergic

1. (adjective). Preventing transmission of parasympathetic nerve impulses.
2. (noun). Substance which prevents transmission of parasympathetic nerve impulses.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2014

anticircular elution (anticircular development)

in planar chromatography

The opposite of circular development. Here the sample as well as the mobile phase is applied at the periphery of a circle and both move towards the centre.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 830

anticlined structures

in polymers

See: isomorphous structures *in polymers*

Source:
Purple Book, p. 43

anticodon

A sequence of three nucleotides in the anticodon-loop of a *t*RNA, which recognizes and binds the complementary triplet sequence (codon) of the mRNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 146

anticyclone

in atmospheric chemistry

A large system of winds that rotate about a centre of high atmospheric pressure, clockwise (viewed from above) in the northern hemisphere and counterclockwise in the southern hemisphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

antiferromagnetic transition

See: ferroic transition, magnetic transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 579

antigen

A substance that stimulates the immune system to produce a set of specific antibodies and that combines with the antibody through a specific binding site or epitope.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 146

antimetabolite

Substance, structurally similar to a metabolite, which competes with it or replaces it, and so prevents or reduces its normal utilization.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2015

antimony–xenon lamp (arc)

An intense source of ultraviolet, visible, and near infra-red radiation produced by an electrical discharge in a mixture of antimony vapour and xenon under high pressure. Its output in the ultraviolet region is higher than that of the mercury–xenon arc.
See: lamp

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2228

antimycotic

Synonym: fungicide

Substance used to kill a fungus or to inhibit its growth. Synonymous with fungicide.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2015

antiparticle

Of a given particle, a particle with the same rest mass, where the two can annihilate.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

antipodes [obsolete]

Obsolete synonym for enantiomers. (Usage strongly discouraged).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2199

antiprismo-

An affix used in names to denote eight atoms bound into a rectangular antiprism.

Source:
Red Book, p. 245
Blue Book, p. 464

antiresistant

Substance used as an additive to a pesticide formulation in order to reduce the resistance of insects to the pesticide.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2015

antiserum

Serum containing antibodies to a particular antigen either because of immunization or after an infectious disease.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2015

antisymmetry principle

The postulate that electrons must be described by wavefunctions which are antisymmetric with respect to interchange of the coordinates (including spin) of a pair of electrons. A corollary of the principle is the Pauli exclusion principle. All particles with half-integral spin (fermions) are described by antisymmetric wavefunctions, and all particles with zero or integral spin (bosons) are described by symmetric wavefunctions.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1923

ap

See: torsion angle

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2199

apex current

Also contains definitions of: apex, apex potential

In measurement of non-faradaic admittance (or tensammetry), a plot of alternating current against applied potential shows a minimum or maximum when a non-electroactive substance undergoes adsorption or desorption at the surface of the indicator electrode. Such a maximum or minimum may be called an apex to emphasize its non-faradaic origin and distinguish it from a 'summit', which would result from a charge-transfer process. The highest value of the current on such an apex may be called an apex current, and the corresponding applied potential may be called an apex potential.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1494

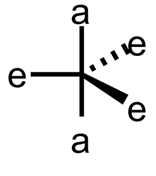
aphicide

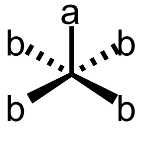
Substance intended to kill aphids.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2015

apical (basal, equatorial)

In trigonal bipyramidal structures (e.g. a five-coordinate trigonal bipyramid with phosphorus as central atom) the term apical refers to the two positions that are collinear with the central atom or to the bonds linking these positions to the central atom. The three equivalent bonds (or positions) in a plane passing through the central atom and perpendicular to the direction of the apical bonds are described as equatorial. (See axial, equatorial for alternative use). The term apical is also used for the bond pointing from the atom at or near the centre of the base to the apex of a pyramidal structure. The positions at or near the base of the pyramid, or the bonds linking those positions to the central atom of the base are described as basal. The apical bonds have also been called axial.





a = apical
b = basal
e = equatorial

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2199

apicophilicity

In trigonal bipyramidal structures with a five-coordinate central atom, the stabilization achieved through a ligand changing its position from equatorial to apical (axial). The apicophilicity of an atom or a group is evaluated by either the energy difference between the stereoisomers (permutational isomers) containing the ligand in apical and equatorial positions or the energy barrier to permutational isomerization (see also Berry pseudorotation). In general, the greater the electronegativity and the stronger the π-electron-withdrawing properties of a ligand (as for Cl, F, CN), the higher is its apicophilicity. The notion of apicophilicity has been extended to four-coordinate bisphenoidal and three-coordinate T-shaped structures, which can be viewed as trigonal bipyramidal species where, respectively, one or two vertices are occupied by phantom ligands (lone electron pairs).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1923

apo-

in carotenoid nomenclature

An unitalicized prefix, preceded by a locant, used to indicate that all of the molecule beyond the carbon atom corresponding to that locant has been replaced by hydrogen atoms.

Source:
White Book, p. 230

apoenzyme

The protein part of an enzyme without the cofactor necessary for catalysis. The cofactor can be a metal ion, an organic molecule (coenzyme), or a combination of both.

Source:
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

apoprotein

A protein without its characteristic prosthetic group or metal.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1257

apoptosis

Active process of programmed cell death requiring metabolic energy, often characterised by fragmentation of DNA, and without associated inflammation.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1039

apparent lifetime

See: lifetime

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2228

apparent (quantity)

A term, indicated by a superscript ', which means that a process is not well known or that its value carries uncertainties which are not known, e.g. $\Delta G^{\mathrm{o}\,\prime}$ is the apparent standard Gibbs energy change. In the context of partial molar quantities the word is used in a different sense; as a symbol for 'apparent' in this connection the use of subscript φ, as in Y_{φ}, is recommended. Other notations employed for this property include ${}^{\varphi}X$ and φ_X.

Source:
PAC, 1986, *58*, 1405 *(Recommendations for the presentation of thermodynamic and related data in biology (Recommendations 1985))* on page 1408

apparent viscosity

of a liquid

The ratio of stress to rate of strain, calculated from measurements of forces and velocities as though the liquid were Newtonian. If the liquid is actually non-Newtonian, the apparent viscosity depends on the type and dimensions of the apparatus used.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

appearance energy (appearance potential)

Refers to ionization of a molecule or atom by electron collision or photon absorption. In mass spectrometry it has often been reported as the voltage which corresponds to the minimum energy of the electrons in the ionizing beam necessary for the production of a given fragment ion. In photoionization it is the minimum energy of the quantum of light which produces ionization of the absorbing molecule.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

appearance potential [obsolete]

See: appearance energy

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

appearance temperature, T_{app}

in electrothermal atomization

The temperature of the atomization surface at which the analyte signal/noise (S/N) ratio reaches a value of 3 when the quantity of analyte in the atomizer is one hundred times the characteristic mass for peak high absorption.

Source:
PAC, 1992, *64*, 253 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XII. Terms related to electrothermal atomization (IUPAC Recommendations 1992))* on page 257

applied potential

The difference of potential measured between identical metallic leads to two electrodes of a cell. The applied potential is divided into two electrode potentials, each of which is the difference of potential existing between the bulk of the solution and the interior of the conducting material of the electrode, an $i\,R$ or ohmic potential drop through the solution, and another ohmic potential drop through each electrode. In the electroanalytical literature this quantity has often been denoted by the term voltage, whose continued use is not recommended.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1502

aprotic (solvent)

Non-protogenic (in a given situation). (With extremely strong Brønsted acids or bases, solvents that are normally aprotic may accept or lose a proton. For example, acetonitrile is in most instances an aprotic solvent, but it is protophilic in the presence of concentrated sulfuric acid and protogenic in the presence of potassium *tert*-butoxide. Similar considerations apply to benzene, trichloromethane, etc.)
See also: dipolar aprotic solvent

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1085

aquagel

Hydrogel in which the network component is a colloidal network.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1807

aquation

The incorporation of one or more integral molecules of water into another species with or without displacement of one or more other atoms or groups. For example, the incorporation of water into the inner ligand sphere of an inorganic complex is an aquation reaction.
See also: hydration

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1086

arachno-

An affix used in names to designate a boron structure intermediate between *nido*- and *hypho*- in degree of openness.

Source:
Red Book, p. 245

Archibald's method

A sedimentation method based on the fact that at the meniscus and at the bottom of the centrifuge cell there is never a flux of the solute across a plane perpendicular to the radial direction and the equations characterizing the sedimentation equilibrium always apply there, even though the system as a whole may be far from equilibrium. The use of the term 'approach to sedimentation equilibrium' for Archibald's method is discouraged, since it has a more general meaning.

Source:
Purple Book, p. 62

area

of an electrode-solution interface

This is understood to be the geometrical or projected area, and to ignore surface roughness.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1493

area of interface

In all measurements it is desirable that quantities like the charge and the capacity be related to unit, true, surface area of the interface. While this is relatively simple for a liquid-liquid interface, there are great difficulties when one phase is solid. In any report of these quantities it is essential to give a clear statement as to whether they refer to the true or the apparent (geometric) area and, especially if the former is used, precisely how it was measured.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 509

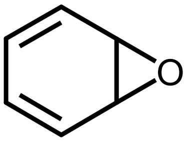
areic

Attribute to a physical quantity obtained by division by area. Areic charge is the charge on a surface divided by the surface area.

Source:
ISO 31-0: 1992 *(Quantities and Units - Part 0: General Principles, Units and Symbols.)*
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 962

arene epoxides

Epoxides derived from arenes by 1,2-addition of an oxygen atom to a formal double bond, e.g. 5,6-epoxycyclohexa-1,3-diene.



(Common usage has extended the term to include examples with the epoxy group bridging nonadjacent atoms.)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318

arene oxides

See: arene epoxides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318

arenes

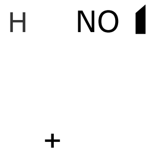
Monoyclic and polycyclic aromatic hydrocarbons.
See: aromatic compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318

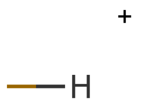
arenium ions

Cations derived formally by the addition of a hydron or other cationic species to any position of an arene, e.g. $C_6H_7^+$, benzenium. The term includes:

1. Arenium σ-adducts (Wheland intermediates) (which are considered to be intermediates in electrophilic aromatic substitution reactions) and other cyclohexadienyl cations.



2. Arenium π-adducts, such as:



[σ-adduct (sigma-adduct), π-adduct (pi-adduct)].
See: aryl cations

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1318

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1077

arenols

Synonymous with phenols (but rarely used).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1319

arenonium ions [obsolete]

An obsolescent name for arenium ions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1319

argon ion laser

A CW or pulsed laser emitting lines from 334 to $529\ \mathrm{nm}$ from singly ionized argon. Principal emissions are at 488.0 and $514.5\ \mathrm{nm}$.
See: gas lasers

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2228

arithmetic mean (average)

The sum of a series of observations divided by the number of observations. Symbol: $\bar{x}$. It can be calculated by the formula:

$$\bar{x} = \frac{\sum x_i}{n}$$

Note:
All summations are taken from 1 to n. Note that the arithmetic mean is an unbiased estimate of the population mean, i.e. μ is the limiting value for $\bar{x}$, as $n \rightarrow \infty$.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 599

aromatic

1. In the traditional sense, 'having a chemistry typified by benzene'.
2. A cyclically conjugated molecular entity with a stability (due to delocalization) significantly greater than that of a hypothetical localized structure (e.g. Kekulé structure) is said to possess aromatic character. If the structure is of higher energy (less stable) than such a hypothetical classical structure, the molecular entity is 'antiaromatic'. The most widely used method for determining aromaticity is the observation of diatropicity in the ^{1}H NMR spectrum.
   See also: Hückel ($4n + 2$) rule, Möbius aromaticity
3. The terms aromatic and antiaromatic have been extended to describe the stabilization or destabilization of transition states of pericyclic reactions The hypothetical reference structure is here less clearly defined, and use of the term is based on application of the Hückel ($4n + 2$) rule and on consideration of the topology of orbital overlap in the transition state. Reactions of

molecules in the ground state involving antiaromatic transition states proceed, if at all, much less easily than those involving aromatic transition states.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1086

See also:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1319

aromatic photocycloaddition

Inter- and intramolecular *photochemical processes* involving the addition of a C–C double (or triple) bond to (i) to the 1,2-positions of an arene in which case it is called an *ortho photocycloaddition*, with formation of a benzocyclobutene (or a benzocyclobutadiene) derivative, (ii) to the 1,3-positions of an arene in which case it is called a *meta photocycloaddition*, with formation of tricyclo[3.3.0.0^{2,8}]oct-3-ene (or octa-3,6-dien) derivatives, or (iii) to the 1,4-positions of an arene in which case it is called a *para photocycloaddition*, with formation of bicyclo[2,2,2]oct-2-ene (or octa-2,5-dien) derivatives.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 303

aromaticity

The concept of spatial and electronic structure of cyclic molecular systems displaying the effects of cyclic electron delocalization which provide for their enhanced thermodynamic stability (relative to acyclic structural analogues) and tendency to retain the structural type in the course of chemical transformations. A quantitative assessment of the degree of aromaticity is given by the value of the resonance energy. It may also be evaluated by the energies of relevant isodesmic and homodesmotic reactions. Along with energetic criteria of aromaticity, important and complementary are also a structural criterion (the lesser the alternation of bond lengths in the rings, the greater is the aromaticity of the molecule) and a magnetic criterion (existence of the diamagnetic ring current induced in a conjugated cyclic molecule by an external magnetic field and manifested by an exaltation and anisotropy of magnetic susceptibility). Although originally introduced for characterization of peculiar properties of cyclic conjugated hydrocarbons and their ions, the concept of aromaticity has been extended to their homoderivatives (see homoaromaticity), conjugated heterocyclic compounds (heteroaromaticity), saturated cyclic compounds (σ-aromaticity) as well as to three-dimensional organic and organometallic compounds (three-dimensional aromaticity). A common feature of the electronic structure inherent in all aromatic molecules is the close nature of their valence electron shells, *i.e.*, double electron occupation of all bonding MOs with all antibonding and delocalized nonbonding MOs unfilled. The notion of aromaticity is applied also to transition states.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1923

arrester

in atmospheric chemistry

Equipment designed to remove particles from a gaseous medium.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

Arrhenius equation

An equation that represents the dependence of the rate constant k of a reaction on the absolute temperature T:

$$k = A\,\mathrm{e}^{\frac{-E_\mathrm{a}}{R\,T}}$$

In its original form the pre-exponential factor A and the activation energy E_a are considered to be temperature-independent.
See also: modified Arrhenius equation

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 153
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1086
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

arsanes

The saturated hydrides of tervalent arsenic, having the general formula As_nH_{n+2}. Individual members having an unbranched arsenic chain are named arsane, diarsane, triarsane, etc. The name of a saturated hydride of arsenic where one or more arsenic atoms have bonding number 5 is formed by prefixing locants and λ^5 symbols to the name of the corresponding arsane, e.g. $H_2AsAsHAsH_2$ triarsane, $H_4AsAsH_3AsH_4$ $1\lambda^5,2\lambda^5,3\lambda^5$-triarsane. Hydrocarbyl derivatives of AsH_3 belong to the class arsines.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1319

arsanylidenes

Synonym: arsinidenes

Recommended name for carbene analogues having the structure R–As: (former IUPAC name is arsinediyls). A common non-IUPAC synonym is arsinidenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1319

arsanylium ions

The arsanyl cation, H_2As^+, and derivatives by substitution. The name arsinylium (systematically derived from arsine) is not applied as it already designates $H_2As(=O)^+$, the acylium ion derived from arsinic acid.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1319

arsenides

Compounds obtained from arsines AsR_3 by replacing one or more hydrogen atoms by a metal, e.g. CaAsPh calcium phenylarsenide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1319

arsine oxides

$H_3As{=}O$ and its hydrocarbyl derivatives. (analogously arsine imides and arsine sulfides), e.g. $(CH_3)_3As{=}O$ trimethylarsine oxide or trimethylarsane oxide.
See: imides (2).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1319

arsines

AsH_3 and compounds derived from it by substituting one, two or three hydrogen atoms by hydrocarbyl groups: R_3As, $RAsH_2$, R_2AsH, R_3As ($R \neq H$) are called primary, secondary and tertiary arsines, respectively. A specific arsine is preferably named as a substituted arsane, e.g. $CH_3CH_2AsH_2$ ethylarsane.
See: arsanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1319

arsinic acids

$H_2As(=O)OH$ and its As-hydrocarbyl derivatives, e.g. $Me_2As(=O)OH$, dimethylarsinic acid.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

arsinous acids

H_2AsOH and its As-hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

arsonic acids

$HAs(=O)(OH)_2$ and its As-hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

arsonium compounds

Salts (including hydroxides) $[R_4As]^+X^-$ containing tetracoordinate arsonium ion and the associated anion.
See also: onium compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

arsonous acids

$HAs(OH)_2$ and its As-hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

arsoranes

The mononuclear hydride AsH_5, systematically named λ^5-arsane, and its hydrocarbyl derivatives. By extension the term also applies to arsonium ylides.
See: ylides, arsanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

artificial graphite [obsolete]

A term often used in place of synthetic graphite

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 477

artificial neural networks

Artificial neural networks (ANN) are algorithms simulating the functioning of human neurons and may be used for pattern recognition problems, *e.g.*, to establish quantitative structure-activity relationships.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1140

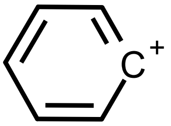
artificial radioactivity

Synonymous with induced radioactivity.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

aryl cations

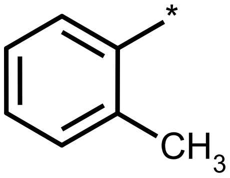
Carbocations formally derived by removal of a hydride ion from a ring carbon atom of an arene.
See: arenium ions, e.g. phenyl cation or phenylium:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

aryl groups

Groups derived from arenes by removal of a hydrogen atom from a ring carbon atom. Groups similarly derived from heteroarenes are sometimes subsumed in this definition. E.g. *o*-tolyl:

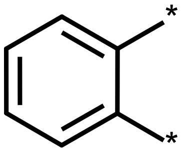


See: heteroaryl groups

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

arylene groups

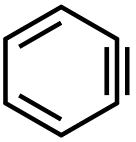
Bivalent groups derived from arenes by removal of a hydrogen atom from two ring carbon atoms. A synonym is arenediyl groups. E.g. *o*-phenylene or benzene-1,2-diyl:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

aryne

A hydrocarbon derived from an arene by abstraction of two hydrogen atoms from adjacent carbon atoms; thus 1,2-didehydroarene. Arynes are commonly represented with a formal triple bond. The analogous heterocyclic compounds are called heteroarynes or hetarynes. For example, benzyne:



Arynes are usually transient species.
See also: benzynes, dehydroarenes, heteroarynes

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1086
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

ascending elution (ascending development)

in planar chromatography

A mode of operation in which the paper or plate is in a vertical or slanted position and the mobile phase is supplied to its lower edge; the upward movement depends on capillary action.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 829

ash

in atmospheric chemistry

The solid residue which remains after the combustion of a fuel such as coal. Ash consists largely of heat treated mineral matter, but it may contain some products of the incomplete combustion of the fuel as well.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

ashing

in analysis

Dry or wet mineralization as a method of preconcentration of trace substances.
See also: charring

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1200

aspirator

Any apparatus that produces a movement of a fluid by suction (e.g. a squeeze bulb, pump, Venturi, etc.)

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

assay

A set of operations having the object of determining the value of a quantity. In analytical chemistry, this term is synonymous with measurement.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515

PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2016

assay kit

A set of components (reagents and other necessary materials) and procedural instructions packaged together and designed for the estimation in vitro of a value of a specified quantity, when used according to the instructions.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515

association

The assembling of separate molecular entities into any aggregate, especially of oppositely charged free ions into ion pairs or larger and not necessarily well-defined clusters of ions held together by electrostatic attraction. The term signifies the reverse of dissociation, but is not commonly used for the formation of definite adducts by colligation or coordination.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1086

association reaction (associative combination)

in mass spectrometry

The reaction of a (slow moving) ion with a neutral species wherein the reactants combine to form a single ionized species.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

associative ionization

in mass spectrometry

This occurs when two excited gaseous atoms or molecular moieties interact and the sum of their internal energies is sufficient to produce a single, additive ionic product.
See also: chemi-ionization

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

asym-

An affix used in names to denote asymmetrical.

Source:
Red Book, p. 245
Blue Book, p. 464

asymmetric

Lacking all symmetry elements (other than the trivial one of a one-fold axis of symmetry), i.e. belonging to the symmetry point group C_1. The term has been used loosely (and incorrectly) to describe the absence of a rotation–reflection axis (alternating axis) in a molecule, i.e. as meaning chiral, and this usage persists in the traditional terms asymmetric carbon atom, asymmetric synthesis, asymmetric induction, etc.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2199
Blue Book, p. 480

asymmetric carbon atom

The traditional name (van't Hoff) for a carbon atom that is attached to four different entities (atoms or groups), e.g. Cabcd.
See also: chirality centre

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2200
Blue Book, p. 480

asymmetric centre

See: chirality centre

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2200

asymmetric destruction

See: kinetic resolution

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2200

asymmetric film

A film bounded by two different bulk phases. When the bulk phases are identical the film is described as symmetric.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1671

asymmetric induction

The traditional term describing the preferential formation in a chemical reaction of one enantiomer or diastereoisomer over the other as a result of the influence of a chiral feature present in the substrate, reagent, catalyst or environment.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2200
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1086

asymmetric membrane

Membrane constituted of two or more structural planes of non-identical morphologies.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1481

asymmetric photochemistry

Photochemical process leading to a chiral substance from an achiral precursor such that one enantiomer predominates over the other.
Note:
Asymmetric induction may be achieved by the use of chiral reagents, a chiral environment, or circularly polarized light.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 304

asymmetric synthesis

A traditional term used for stereoselective synthesis of chiral compounds.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2200

asymmetric transformation

Also contains definition of: deracemization

The conversion of a racemate into a pure enantiomer or into a mixture in which one enantiomer is present in excess, or of a diastereoisomeric mixture into a single diastereoisomer or into a mixture in which one diastereoisomer predominates. This is sometimes called deracemization. If the two enantiomers of a chiral substrate A are freely interconvertible and if an equal amount or excess of a non-racemizing second enantiomerically pure chemical species, say (*R*)-B, is added to a solution of racemic A, then the resulting equilibrium mixture of adducts A • B will, in general, contain unequal amounts of the diastereoisomers (*R*)-A • (*R*)-B and (*S*)-A • (*R*)-B. The result of this equilibration is called asymmetric transformation of the first kind. If, in such a system, the two diastereoisomeric adducts differ considerably in solubility so that only one of them, say (*R*)-A • (*R*)-B, crystallizes from the solution, then the equilibration of diastereoisomers in solution and concurrent crystallization will continue so that all (or most) of the substrate A can be isolated as the crystalline diastereoisomer (*R*)-A • (*R*)-B. Such a 'crystallization-induced asymmetric transformation' is called an asymmetric transformation of the second kind.
See also: stereoconvergence

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2200

asymmetry

Denoting absence of any symmetry.

Source:
Blue Book, p. 479

asymmetry potential

of a glass electrode

The measured potential difference of a symmetrical cell with identical solutions and reference electrodes on each side of the glass membrane. There is rarely the need, nor the possibility, of measuring the asymmetry potential of commercial glass electrodes. Drifts in glass electrode potentials with time and variations from day-to-day in the potential measured in a standard buffer may be attributed to changes in asymmetry potential.

Source:
Orange Book, p. 27

atactic macromolecule

A regular macromolecule in which the configurational (base) units are not all identical.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2292

atactic polymer

A polymer composed of atactic macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2303

atmosphere

Non-SI unit of pressure, $1\ \mathrm{atm} = 101\ 325\ \mathrm{Pa}$.

Source:
Green Book, 2nd ed., p. 112
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 962

atmosphere

of the earth

The entire mass of air surrounding the earth which is composed largely of nitrogen, oxygen, water vapour, clouds (liquid or solid water), carbon dioxide, together with trace gases and aerosols.
See: composition of pure air

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

atmospheric pressure ionization [obsolete]

in mass spectrometry

An ambiguous term; in essence, it is used to describe chemical ionization at atmospheric pressure. It is recommended that use of the term be discontinued.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

atom

Smallest particle still characterizing a chemical element. It consists of a nucleus of a positive charge (Z is the proton number and e the elementary charge) carrying almost all its mass (more than 99.9%) and Z electrons determining its size.

Source:
Physical Chemistry Division, unpublished

Red Book, p. 35

atom-atom polarizability

A quantity used in perturbation *HMO* theory as a measure of the change in electron density, q, of atom s caused by a change in the electronegativity (or Coulomb integral) of atom r:

$$\pi_{\mathrm{sr}} = \frac{\partial q_{\mathrm{s}}}{\partial a_{\mathrm{r}}}$$

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1924

atom-bond polarizability

A quantity used in perturbation *HMO* theory as a measure of the change in electron density, q, of atom m caused by a change in the resonance integral, β, of bond rs:

$$\pi_{\mathrm{m,rs}} = \frac{\partial q_{\mathrm{m}}}{\partial \beta_{\mathrm{rs}}}$$

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1924

atomic charge

The charge attributed to an atom A within a molecule defined as $\zeta = Z_{\mathrm{A}} - q_{\mathrm{A}}$, where Z_{A} is the atomic number of A and q_{A} is the electron density assigned to A. The method of calculation of q_{A} depends on the choice of the scheme of partitioning electron density. In the framework of the Mulliken population analysis q_{A} is associated with the so-called gross atomic population: $q_{\mathrm{A}} = \sum q_{\mu}$, where q_{μ} is a gross population for an orbital μ in the basis set employed defined according to

$$q_{\mu} = P_{\mu\mu} + \sum_{\nu \neq \mu} P_{\mu\nu} S_{\mu\nu}$$

where $P_{\mu\nu}$ and $S_{\mu\nu}$ are the elements of density matrix and overlap matrix, respectively (see overlap integral). In the Hückel molecular orbital theory (where $S_{\mu\nu} = \delta_{\mu\nu}$), $q_{\mu} = n_{\mu} P_{\mu\mu}$, where n_{μ} is the number of electrons in the MO μ.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1924

atomic fluorescence

A combined process of photon absorption by an atom followed by spontaneous photon emission.

Source:
Orange Book, p. 121

atomic laser

A gas laser which is pumped using energy transfer from other atoms or molecules. Examples are the helium-neon (He Ne) the copper vapour laser.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1919

atomic mass constant

One twelfth of the mass of a carbon-12 atom in its nuclear and electronic ground state, $m_{\mathrm{u}} = 1.660\ 5402(10) \times 10^{-27}\ \mathrm{kg}$. It is equal to the unified atomic mass unit

Source:
CODATA Bull. 1986, *63*, 1
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 962

atomic mass m_{a}

Rest mass of an atom in its ground state. The commonly used unit is the unified atomic mass unit.

Source:
Green Book, 2nd ed., p. 20
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 962

atomic mass unit

See: unified atomic mass unit

Source:
CODATA Bull. 1986, *63*, 1
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 962

atomic number, Z

Also contains definition of: proton number

The number of protons in the atomic nucleus.

Source:
Green Book, 2nd ed., p. 20
Red Book, p. 35
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 962

atomic orbital, ψ, φ, χ

One-electron wavefunction obtained as a solution of the Schrödinger equation for an atom.

Source:
Green Book, 2nd ed., p. 19
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1086

atomic spectral lines

Also contains definition of: ionic spectral lines

Atomic and ionic spectral lines originate from specified electronic transitions between energy levels of atoms and ions, respectively. In the past it has been common useage to denote atomic lines as arc lines and ionic lines as spark lines. This usage is now considered to be incorrect. The correct way to indicate that lines are due to atomic or ionic transitions is: Element symbol I wavelength e.g. Cu I $324.7\ \mathrm{nm}$; and Element symbol II wavelength e.g. Cu II $213.6\ \mathrm{nm}$. Similarly for higher states of ionization, the type of line is represented by III, IV, etc.
See also: ionic spectral lines

Source:
Orange Book, p. 118

atomic symbol

One, two or three letters used to represent the atom in chemical formulae.

Source:
Red Book, p. 36

atomic units

The units designed to simplify the form of the fundamental equations of quantum mechanics by eliminating from them fundamental constants. The atomic unit of length is the Bohr radius, $a_{\mathrm{o}} = \frac{h^2}{4\,\pi^2\,m\,e^2} = 5.291\ 77249 \times 10^{-11}\ \mathrm{m}\ \ (0.529177249\ \mathrm{Å})$. Energy is measured in hartrees, where $1\ \mathrm{hartree} = \frac{e^2}{a_{\mathrm{o}}} = 4.359\ 7482 \times 10^{-18}\ \mathrm{J}$. Masses are specified in terms of atomic mass unit, $\mathrm{amu} = 1.6605402 \times 10^{-27}\ \mathrm{kg}$ and of the electron mass unit, $m_{\mathrm{e}} = 0.910953 \times 10^{-30}\ \mathrm{kg}$. The advantage of atomic units is that if all calculations are directly expressed in such units, the results do not vary with any revision of the numerical values of the fundamental constants.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1924

atomic weight

See: relative atomic mass

Source:
Green Book, 2nd ed., p. 41
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 962

atomization

in analytical flame spectroscopy

The conversion of volatilized analyte into free atoms.

Source:
Orange Book, p. 165

atomization surface temperature, T_s

in electrothermal atomization

The temperature of the support from which the sample is atomized.

Source:
PAC, 1992, *64*, 253 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XII. Terms related to electrothermal atomization (IUPAC Recommendations 1992))* on page 257

atomize

To subdivide a liquid into very small particles; methods include: impact with a jet of gas, use of a spinning disk generator, vibrating orifice generator, etc.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

atomizer

in analytical flame spectroscopy

Any system which is capable of converting the analyte into atomic vapour.

Source:
Orange Book, p. 165

atom–molecule complex mechanism

A mechanism that sometimes applies to the combination of atoms, but rarely of free radicals. In this mechanism the atom A first combines with a third body or chaperon,

$$\mathrm{A} + \mathrm{M} \longrightarrow \mathrm{AM}$$

,

and the complex AM then forms $A_2 + M$ by collision with another atom A.
Contrast the energy-transfer mechanism.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 153

atropisomers

A subclass of conformers which can be isolated as separate chemical species and which arise from restricted rotation about a single bond, e.g. *ortho*-substituted biphenyl, 1,1,2,2-tetra-*tert*-butylethane.
See: rotational barrier

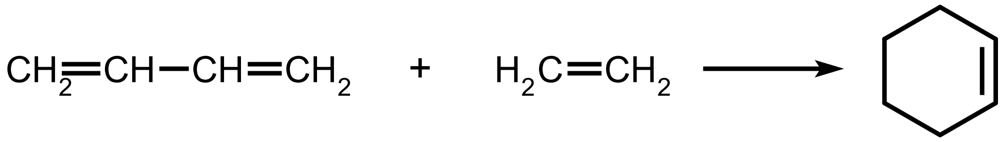
Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2200

attachment

A transformation by which one molecular entity (the substrate) is converted into another by the formation of one (and only one) two-centre bond between the substrate and another molecular entity and which involves no other changes in connectivity in the substrate. For example, the formation of an acyl cation by attachment of carbon monoxide to a carbenium ion (R^+):

$$\mathrm{R}^{+} + \mathrm{CO} \longrightarrow (\mathrm{RCO})^{+}$$

The product of an attachment may also be the adduct of the two reactants, but not all adducts can be represented as the products of an attachment. (For example, the Diels–Alder cycloaddition:



results in an adduct of buta-1,3-diene and ethene, but the reaction cannot be described as an attachment since bonds are formed between more than two centres.)
See also: colligation, electron attachment

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1086

attenuance, *D*

Analogous to absorbance, but taking into account also the effects due to scattering and luminescence. It was formerly called extinction.

Source:
Green Book, 2nd ed., p. 32

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2228
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 962

attenuance filter

Synonym: neutral-density filter

An optical device (filter) which reduces the radiant power of a light beam by a constant factor over all wavelengths within its operating range. Sometimes called attenuator or neutral density filter.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2229

attenuation

The reduction of a radiation quantity upon passage of radiation through matter resulting from interactions of the radiation with the matter it traverses.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

attenuation coefficient

Analogous to absorption coefficient but taking into account also the effects due to scattering and luminescence. It was formerly called extinction coefficient.

Source:
Green Book, 2nd ed., p. 32

See also:
Orange Book, p. 212
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 963

atto

SI prefix for 10^{-18} (symbol: a).

Source:
Green Book, 2nd ed., p. 74

attractive potential-energy surface

Also contains definition of: early-downhill surface

A potential-energy surface for a process **A + B–C** in which the initial descent of the system into the product valley is associated with a substantial decrease in the **A–B** distance and with little separation between the products **A–B** and **C**. In terms of a potential-energy profile, the energy barrier occurs in the early stage of the reaction path. Attractive surfaces are also called early-downhill surfaces, and the barrier in such a surface is called a Type-I barrier.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 153

attractive–mixed–repulsive (AMR) classification

A classification of potential-energy surfaces in which a highly attractive surface is at one extreme and a highly repulsive surface is at the other. The energy release in intermediate cases is referred to as mixed.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 153

attributable risk

Part of a risk that is identified as due to exposure to a defined substance.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1039

aufbau principle

A rule for building up the electronic configuration of atoms and molecules. It states that a maximum of two electrons are put into orbitals in the order of increasing orbital energy: the lowest-energy orbitals are filled before electrons are placed in higher-energy orbitals.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1925

Auger effect

The emission of an electron from an atom accompanying the filling of a vacancy in an inner electron shell.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

Auger electron

Electron originating in the Auger effect.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

See also:
PAC, 1980, *52*, 2541 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - IV X-ray emission spectroscopy)* on page 2546

Auger electron spectroscopy

Any technique in which a specimen is bombarded with keV-energy electrons or X-rays, and the energy distribution of the electrons produced through radiationless de-excitation of the atoms in the sample (Auger electrons) is recorded. The derivative curve may also be recorded.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2025

Auger electron yield

The fraction of the atoms having a vacancy in an inner orbital which relax by emission of an Auger electron.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

Auger yield

For a given excited state of a specified atom the probability that the de-excitation occurs by the Auger effect.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

autacoid

A biological substance secreted by various cells whose physiological activity is restricted to the vicinity of its release; it is often referred to as a local hormone.

Source:
PAC, 1998, *70*, 1129 *(Glossary of terms used in medicinal chemistry (IUPAC Recommendations 1998))* on page 1129

auto-ionization

in mass spectrometry

This occurs when an internally supra-excited atom or molecular moiety loses an electron spontaneously without further interaction with an energy source. (The state of the atom or molecular moiety is known as a pre-ionization state.)

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547
Orange Book, p. 206

autocatalytic reaction

A chemical reaction in which a product (or a reaction intermediate) also functions as a catalyst. In such a reaction the observed rate of reaction is often found to increase with time from its initial value.
See: order of reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1087
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2292

automation

in analysis

Mechanization with process control, where process means a sequence of manipulations. One or several functions in an analytical instrument may be automated. The corresponding adjective is automated and the verb is automate.
See also: mechanization

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1659

automerization

Synonymous with degenerate rearrangement.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1087

autophobicity

If adsorption equilibrium and mutual saturation of the phases is not achieved instantly, it is possible to distinguish the initial spreading tension, $\sigma_{\mathrm{i}}^{\alpha\beta\delta}$, from the final spreading tension, $\sigma_{\mathrm{f}}^{\alpha\beta\delta}$, when equilibrium has been reached. In the case in which $\sigma_{\mathrm{i}}^{\alpha\beta\delta}$ is positive, while $\sigma_{\mathrm{f}}^{\alpha\beta\delta}$ is negative, the system is said to exhibit autophobicity.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 598

autoprotolysis

A proton (hydron) transfer reaction between two identical molecules (usually a solvent), one acting as a Brønsted acid and the other as a Brønsted base. For example:

$$2H_2O \longrightarrow H_3O^+ + OH^-$$

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1087

autoprotolysis constant

The product of the activities (or, more approximately, concentrations) of the species produced as the result of autoprotolysis. For solvents in which no other ionization processes are significant the term is synonymous with 'ionic product'. The autoprotolysis constant for water, K_{w}, is equal to the product of activities:

$$a(\mathrm{H_3O^+})\, a(\mathrm{OH^-}) = 1.0 \times 10^{-14}$$

at 25 °C.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1087

autoradiograph

A radiograph of an object containing radioactive substance, produced by placing the object adjacent to a photographic plate or film or a fluorescent screen.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

autoradiolysis

Radiolysis of a radioactive material resulting directly or indirectly from its radioactive decay.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

auxiliary electrode

Three-electrode cells comprise (1) an indicator (or test) electrode or a working electrode, at the surface of which processes that are of interest may occur, (2) a reference electrode and (3) a third electrode, the auxiliary or counter electrode, which serves merely to carry the current flowing through the cell, and at the surface of which no processes of interest occur. If processes of interest occur at both the anode and the cathode of a cell (as in differential amperometry or controlled current potentiometric titration with two indicator electrodes), the cell should be said to comprise two indicator (or test) working electrodes.

Source:
Orange Book, p. 59

auxochrome [obsolete]

An atom or group which, when added to or introduced into a chromophore, causes a bathochromic shift and/or a hyperchromic effect in a given band of the chromophore, usually in that of lowest frequency. This term is obsolete.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2229

auxotrophy

The inability of a organism to synthesize a particular organic compound required for its growth.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 147

average current density

Also contains definition of: local current density

The average current density, j, is defined by

$$j = A^{-1} \int_A j_x \mathrm{d}A$$

where A is the electrode area, j_x is the local current density and dA is an infinitesimal surface element.

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1836

average degree of polymerization

Any average, $\bar{X}_\mathrm{k}$, of the degree of polymerization, where k specifies the type of average.

Source:
Purple Book, p. 55

average life

in nuclear chemistry

Defined for an atom or nuclear system in a specified state. For an exponentially decaying system, it is the average time for the number of atoms or nuclei in a specified state to decrease by a factor e. Synonymous with mean life.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

average rate of flow

in polarography

The ratio of the mass of a drop, at the instant when it is detached from the tip of the capillary, to the drop time t_1; the average value of the instantaneous rate of flow over the entire life of the drop.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1503

Avogadro constant

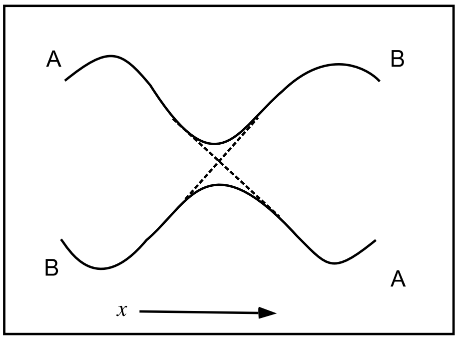
Fundamental physical constant (symbols: L, N_A) representing the molar number of entities: $L = 6.022\ 141\ 79\ \ (30) \times 10^{23}\ \mathrm{mol}^{-1}$.

Source:
CODATA 2006
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 963

avoided crossing

of potential-energy surfaces

Frequently, two Born–Oppenheimer electronic states (A, B) change their energy order as molecular geometry (x) is changed continuously along a path. In the process their energies may become equal at some points (the surfaces are said to cross, dotted lines in the figure), or only come relatively close (the crossing of the surfaces is said to be avoided). If the electronic states are of the same symmetry, the surface crossing is always avoided in diatomics and usually avoided in polyatomics.



Synonymous with intended crossing.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2229

Avrami equation

An equation, describing crystallization kinetics, of the form:

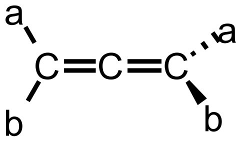
$$1 - \varphi_c = e^{-K t^n}$$

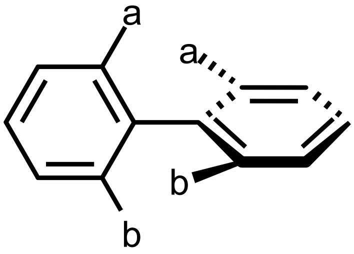
where φ_c is the crystalline volume fraction developed at time t and constant temperature, K and n are suitable parameters. K is temperature dependent. According to the original theory, n should be an integer from 1 to 4, the value of which should depend only on the type of the statistical model; however, it has become customary to regard it as an adjustable parameter that may be non-integral.

Source:
Purple Book, p. 85

axial chirality

Term used to refer to stereoisomerism resulting from the non-planar arrangement of four groups in pairs about a chirality axis. It is exemplified by allenes abC=C=Ccd (or abC=C=Cab) and by the atropisomerism of *ortho*-substituted biphenyls. The configuration in molecular entities possessing axial chirality is specified by the stereodescriptors R_a and S_a (or by P or M).



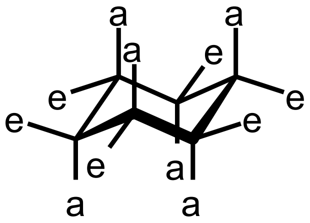


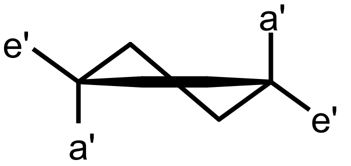
Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2201

axial (equatorial)

Also contains definitions of: pseudo-axial, pseudo-equatorial, quasi-axial, quasi-equatorial

In the chair form of cyclohexane ring bonds to ring atoms (and molecular entities attached to such bonds) are termed axial or equatorial according to whether the bonds make a relatively large or small angle, respectively, with the plane containing or passing closest to a majority of the ring atoms. Thus the axial bonds are approximately parallel to the C_3 axis and the equatorial bonds approximately parallel to two of the ring bonds. These terms are also used for the chair form of other saturated six-membered rings. The corresponding bonds occurring at the allylic positions in mono-unsaturated six-membered rings are termed pseudo-axial (or quasi-axial) and pseudo-equatorial (or quasi-equatorial). The terms axial and equatorial have similarly been used in relation to the puckered conformation of cyclobutane, crown conformer of cyclooctane, etc. and the terms pseudo-axial and pseudo-equatorial in the context of the non-planar structures of cyclopentane and cycloheptane.





a = axial
e = equatorial
a' = pseudo-axial
e' = pseudo-equatorial

See apical (basal, equatorial) for an alternative use of axial and equatorial with bipyramidal structures.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2200

axialite

in polymer crystals

A multilayer aggregate, consisting of lamellar crystals splaying out from a common edge.

Source:
Purple Book, p. 82

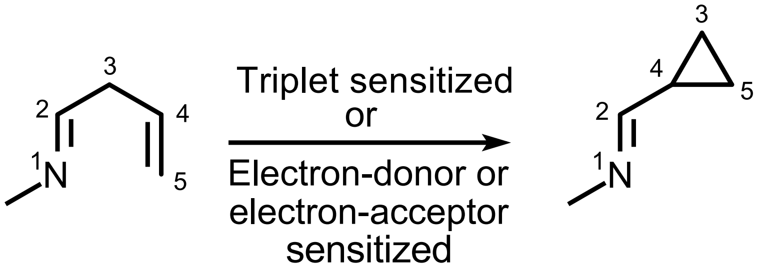
axis of helicity

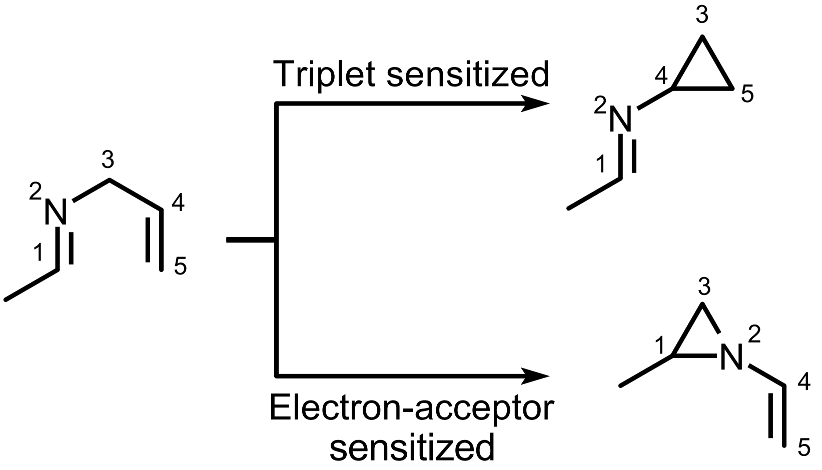
See: helicity

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2201

aza-di-π-methane rearrangement

Photochemical reaction of a 1-aza-1,4-diene or a 2-aza-1,4-diene in the triplet excited state to form the corresponding cyclopropylimine.
Note:
The rearrangement formally amounts to a 1,2-shift of the imino group and 'bond formation' between the C(3) and C(5) carbon atoms of the azadiene skeleton. 1-Aza-1,4-dienes also undergo the rearrangement to cyclopropylimines using electron-acceptor and electron-donor sensitizers via radical-cation and radical-anion intermediates, respectively. 2-Aza-1,4-dienes rearrange to *N*-vinylaziridines on irradiation using electron-acceptor sensitizers. In this instance the reaction amounts to a 1,2-shift of the alkene unit and “bond formation” between the C(1) and C(3) carbon atoms of the azadiene skeleton.





See also: di-π-methane rearrangement, di-π-silane rearrangement, oxa-di-π-methane rearrangement

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 305

azacarbenes [obsolete]

See: nitrenes

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1087

azanes

Saturated acyclic nitrogen hydrides having the general formula N_nH_{n+2} .

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

azenes [obsolete]

See: nitrenes

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1087

azides

1. Compounds bearing the group N_3, viz. $–N=N^+=N^–$; usually attached to carbon, e.g. PhN_3 phenyl azide or azidobenzene.
2. Salts of hydrazoic acid, HN_3, e.g. NaN_3 sodium azide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1320

azimines [obsolete]

A commonly used but undesirable term for azo imides (Should not be confused with 'azimino', the name for the bridging group, –N=N–NH–).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azines

Condensation products, $R_2C=NN=CR_2$, of two moles of a carbonyl compound with one mole of hydrazine (This term should not be confused with the ending -azine appearing in Hantzsch-Widman names for some heterocycles).
See also: aldazines, ketazines

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azinic acids

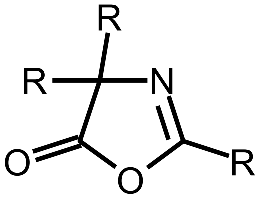
Also contains definition of: nitronic acids

Derivatives of the parent structure $H_2N^+(O^–)OH$, of which the alkylidene derivatives, $R_2C=N^+(O^–)OH$ (tautomers of nitroalkanes), are the most commonly encountered. The alkylideneazinic acids are known as nitronic acids or, synonymously as *aci*-nitro compounds, e.g. $CH_2=N^+(O^–)OH$ methylideneazinic acid.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azlactones

Oxazol-5(4*H*)-ones I, compounds derived by cyclization of *N*-acyl α-amino carboxylic acids, $RC(=O)NHCR_2C(=O)OH$, through formal loss of the elements of water. 4-Hydrocarbylideneazlactones II are often referred to as 'unsaturated azlactones'.



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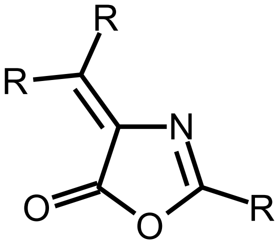


II

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

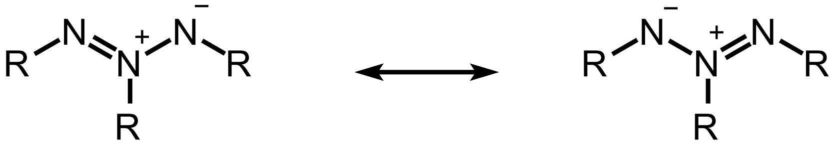
azo compounds

Derivatives of diazene (diimide), HN=NH, wherein both hydrogens are substituted by hydrocarbyl groups, e.g. PhN=NPh azobenzene or diphenyldiazene.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azo imides

N-Imides of azo compounds, analogous to azoxy compounds, having a delocalized structure



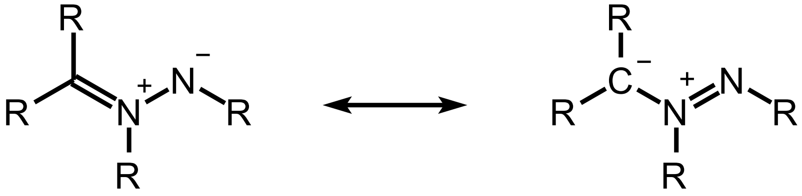
commonly but undesirably referred to as azimines.
See: dipolar compounds, imides (2), ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azomethine imides

Synonym: azo ylides

The 1,3-dipolar N-imides of azomethines having the structure



The term azo ylides, derived from the second resonance form, has also been used.
See: imides (2), ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

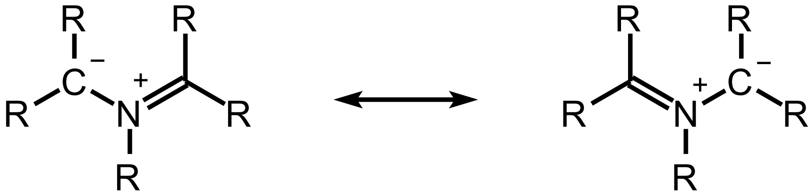
azomethine oxides

Synonymous with nitrones.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azomethine ylides

1,3-Dipolar compounds having the structure



See also: ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azomethines

Compounds having the structure $RN{=}CR_2$ ($R \neq H$). Many consider the term to include the compounds $RN{=}CRH$ ($R \neq H$), thus making azomethines synonymous with Schiff bases.
See: imines

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azonic acids

N-Hydrocarbyl derivatives of the parent structure $HN^+(O^-)(OH)_2$. Cf. phosphonic acids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azoxy compounds

N-Oxides of azo compounds of structure $RN{=}N^+(O^-)R$, e.g. $PhN{=}N^+(O^-)Ph$ azoxybenzene or diphenyldiazene oxide.
See: dipolar compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1321

azylenes [obsolete]

See: nitrenes

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1087

β-cleavage

in mass spectrometry

Fission next but one to a heteroatom or functional group producing a radical and an ion.
See also: α-cleavage

Source:
Orange Book, p. 207

β-decay

Nuclear decay in which a β-particle is emitted or in which orbital electron capture occurs.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

β-particle

Electron ejected from a radioactive nucleus.

Source:
Green Book, 2nd ed., p. 93
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

back donation

Also contains definition of: Chatt–Dewar–Duncanson model

A description of the bonding of π-conjugated ligands to a transition metal which involves a synergic process with donation of electrons from the filled π-orbital or lone electron pair orbital of the ligand into an empty orbital of the metal (donor–acceptor bond), together with release (back donation) of electrons from an *n*d orbital of the metal (which is of π-symmetry with respect to the metal–ligand axis) into the empty π*-antibonding orbital of the ligand.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1925

back electron transfer

A term often used to indicate thermal reversal of excited state electron transfer restoring the donor and acceptor in their original oxidation level. In using this term one should also specify the resulting electronic state of the donor and acceptor.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2229

back extraction

Synonymous with stripping (by extraction).

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2386

back scatter coefficient

in in situ microanalysis

Number of back scattered electrons (BSEs) generated per primary electron for a given specimen and experimental condition. It depends on (mean) atomic number of the excited area of the sample, angle between electron beam and sample surface, primary electron energy and thickness of the sample.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2026

back scattered electrons (BSEs)

in in situ microanalysis

All primary electrons which are scattered out of the original direction and retransmitted through the surface of the solid. In practice, electrons emitted from the surface of a solid under electron bombardment which have a kinetic energy in the range between $50\ \mathrm{eV}$ and excitation energy (E_0).

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2026

back washing [obsolete]

Often used as a synonym for stripping ; the term is not recommended.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2386

backbone

See: main chain

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2294

backflush

Temporary reversal of the direction of the permeable flow.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1487

background concentration (level)

Synonym: baseline concentration *in atmospheric chemistry*

in atmospheric chemistry

The concentration of a given species in a pristine air mass in which anthropogenic impurities of a relatively short lifetime are not present. The background concentrations of relatively long-lived molecules, methane, carbon dioxide, halocarbons (CF_3Cl, CF_2Cl_2, etc.) and some other species continue to rise due to anthropogenic input, so the composition of background air is undergoing continual change. Background concentration of a given species is sometimes considered to be the concentration of that impurity in a given air mass when the contribution from anthropogenic sources under study is absent. Synonymous with baseline concentration.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

background mass spectrum

The mass spectrum observed when no sample is intentionally introduced into the mass spectrometer or spectrograph.

Source:
Orange Book, p. 34

background

of a radiation measuring device

The term employed to designate the value indicated by a radiation measuring device in the absence of the source whose radiation is to be measured, when the device is placed under its normal conditions of operation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

background radiation

1. Radiation from any source other than the one it is desired to detect or measure.

   Source:
   PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516
   Orange Book, p. 213
2. Radiation which originates from the source and reaches the detector when no analyte is present.

   Source:
   PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1462

backscatter

Also contains definition of: forward scattering

Scattering of radiation in a generally backward direction. In the assay of radioactivity, it applies to the scattering of radiation into the radiation detector from any material except the sample and the detector. In light scattering, it is said to occur when the scattering angle, θ, is $180\ °$. Conversely, forward scattering occurs when θ is $0\ °$.

Source:
Orange Book, p. 213
PAC, 1983, *55*, 931 *(Definitions, terminology and symbols in colloid and surface chemistry. Part 1.14: Light scattering (Provisional))* on page 932

baffle chamber

in atmospheric chemistry

A chamber used in incinerator design to promote the settling of fly ash and coarse particulate matter by changing the direction and/or reducing the velocity of the gases produced by the combustion of the refuse.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

bag filter

Also contains definition of: fabric filter

in atmospheric chemistry

A large bag constructed of a suitable fabric which is often tubular in shape, into which a particle-containing air stream flows. Modern bags are constructed of a fabric which is capable of collecting all but very fine particles in the gas stream. The efficiency of the removal of particles of various size ranges changes with the amount of particles captured by the filter and the filtering time. The bag operates on the same principle as the one on a household vacuum cleaner.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2175

baghouse

in atmospheric chemistry

An installation which contains many bag filters in parallel so that the resistance to air flow in a large installation is not seriously increased by the addition of these controls.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

Bainite transition

A term that is sometimes used in metallurgy for the martensitic transition that describes the transition between a face-centred-cubic lattice and a body-centred-tetragonal lattice. Example: The transition between the face-centred-cubic lattice of austenite and the body-centred-tetragonal lattice of a martensite.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 579

baking

in carbon chemistry

The process in which the carbonaceous binder, usually coal tar pitch or petroleum pitch, as part of a shaped carbon mix is converted to carbon yielding a rigid carbon body by the slow application of heat. The process can take as little as $14\ \text{days}$ in coarse-grained, electrothermic grades (low binder level) and as long as $36\ \text{days}$ in ultra-fine-grained, speciality grades (high binder level). The final baking temperature can be in the range of $1100 - 1500\ \text{K}$, depending on the grade.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 477

Baldwin's rules

A set of empirical rules for certain formations of 3- to 7-membered rings. The predicted pathways are those in which the length and nature of the linking chain enables the terminal atoms to achieve the proper geometries for reaction. The disfavoured cases are subject to severe distortions of bond angles and bond distances.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1088

band spectra

The combination of many different spectral lines resulting from vibrational, rotational and electronic transitions. Unresolved band spectra may appear as a spectral continuum.

Source:
Orange Book, p. 118

bandgap energy E_g

The energy difference between the bottom of the conduction band and the top of the valence band in a semiconductor or an insulator.
See: conduction band, Fermi level

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2229

bandpass filter

An optical device which permits the transmission of radiation within a specified wavelength range and does not permit transmission of radiation at higher or lower wavelengths. It can be an interference filter.
See also: cut-off filter

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2229

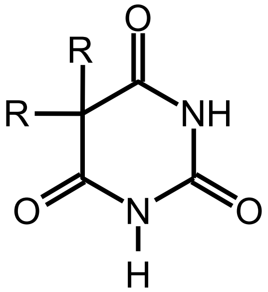
bar

Non-SI unit of pressure, $\mathrm{bar} = 10^5\ \mathrm{Pa}$.

Source:
Green Book, 2nd ed., p. 75
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 963

barbiturates

1. Pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (trivial name barbituric acid) and derivatives:



   (keto tautomeric form)
2. Salts of barbituric acid and its derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322

barn

Non-SI unit of area, $\mathrm{b} = 10^{-28}\ \mathrm{m}^2$, used to express cross sections in nuclear reactions.

Source:
Green Book, 2nd ed., p. 75

Barton reaction

Photolysis of a nitrite to form a δ-nitroso alcohol. The mechanism is believed to involve a homolytic RO–NO cleavage, followed by δ-hydrogen abstraction and radical coupling.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2229

base

A chemical species or molecular entity having an available pair of electrons capable of forming a covalent bond with a hydron (proton) (see Brønsted base) or with the vacant orbital of some other species (see Lewis base).
See also: hard base, superbase

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1088
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

base electrolyte

Synonymous with supporting electrolyte.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1501

base kind of quantity

A kind of quantity considered dimensionally independent of other kinds of quantities, i.e. it is not defined by an equation containing other kinds of quantities, e.g. length, mass, amount of substance.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2459

base pairing

The specific association between two complementary strands of nucleic acids that results from the formation of hydrogen bonds between the base components of the nucleotides of each strand: A=T and G≡C in DNA, A=U and G≡C (and sometimes G=U) in RNA (the lines indicate the number of hydrogen bonds). Single-stranded nucleic acid molecules can adopt a partially double-stranded structure through intrastrand base pairing.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 147

PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2017

base peak

in mass spectrometry

The peak in a mass spectrum corresponding to the separated ion beam which has the greatest intensity. This term may be applied to the spectra of pure substances or mixtures.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1554
Orange Book, p. 206

base quantity

One of the quantities that, in a system of quantities, are conventionally accepted as functionally independent of one another. In the SI, these are: length, mass, time, electric current, temperature, amount of substance, and luminous intensity. All other physical quantities (and units) are regarded as being derived from these base quantities (and base units).

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 963
PAC, 1986, *58*, 1405 *(Recommendations for the presentation of thermodynamic and related data in biology (Recommendations 1985))* on page 1406

base unit

of measurement

Unit of measurement of a base quantity in a given system of quantities. By international agreement, a set of seven dimensionally independent units form the SI base units: the metre, kilogram, second, ampere, kelvin, mole and candela.
See: unit *of measurement*

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 963
PAC, 1986, *58*, 1405 *(Recommendations for the presentation of thermodynamic and related data in biology (Recommendations 1985))* on page 1406

baseline error

in spectrochemical analysis

An error which arises if the two beams in a double-beam spectrometer are not fully equivalent in transmitted power nor are corrected to be so (e.g. due to unmatched cells).

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1456

baseline

in chromatography

The portion of the chromatogram recording the detector response when only the mobile phase emerges from the column.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 834

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

basicity

For Brønsted bases, the tendency of a compound to act as hydron (proton) acceptor. The basicity of a chemical species is normally expressed by the acidity of the conjugate acid (see conjugate acid–base pair). For Lewis bases it relates to the association constants of Lewis adducts and π-adducts.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1088

basis function

A one-electron function used in the expansion of the molecular orbital function. Basis functions are commonly represented by atomic orbitals (see also Slater-type orbital or Gaussian-type orbital) centered on each atom of the molecule.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1925

basis set

A set of basis functions employed for the representation of molecular orbitals. One may distinguish the minimal basis set (includes one basis function for each SCF occupied atomic orbital with distinct principal and angular momentum quantum numbers); split valence basis set (includes two or more sizes of basis function for each valence orbital); double zeta (DZ) basis set (a split valence basis set that includes exactly twice as many functions as the minimal basis set); extended basis set (the set larger than the double zeta basis set); polarized basis set (incorporates basis functions of higher angular quantum number beyond what is required by the atom in its electronic ground state; allows orbitals to change not only a size, but also a shape); basis set with diffuse functions and others.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1925

batch

in analytical chemistry

A quantity of material which is known or assumed to be produced under uniform conditions. Some vocabularies assume 'lot' and 'batch' to be synonymous. The distinction made here with respect to knowledge of production history permits a lot to consist of one or more batches and is useful in interpreting the results of analysis.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1202

batch operation

in analysis

The operation of an analytical instrument in such a way that one or more analytical procedures must be completed for a sequence of samples before the next sequence can be started. This term batch usually implies a sequence of a variably sized group of samples, the size of which is not related to a particular type of instrument.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

batch reactor

In a batch reactor the reactants and the catalyst are placed in the reactor which is then closed to transport of matter and the reaction is allowed to proceed for a given time whereupon the mixture of unreacted material together with the products is withdrawn. Provision for mixing may be required.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

Bates–Guggenheim convention

See: Debye–Hückel equation

Source:
PAC, 1984, *56*, 567 *(Physicochemical quantities and units in clinical chemistry with special emphasis on activities and activity coefficients (Recommendations 1983))* on page 569

bathochromic shift (effect)

Shift of a spectral band to lower frequencies (longer wavelengths) owing to the influence of substitution or a change in environment. It is informally referred to as a red shift and is opposite to hypsochromic shift (blue shift).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1088
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2230

bead-rod model

A model simulating the hydrodynamic properties of a chain macromolecule consisting of a sequence of beads, each of which offers hydrodynamic resistance to the flow of the surrounding medium and is connected to the next bead by a rigid rod which does not. The mutual orientation of the rods is random.

Source:
Purple Book, p. 60

bead-spring model

A model simulating the hydrodynamic properties of a chain macromolecule consisting of a sequence of beads, each of which offers hydrodynamic resistance to the flow of the surrounding medium and is connected to the next bead by a spring which does not contribute to the frictional interaction but which is responsible for the elastic and deformational properties of the chain. The mutual orientation of the springs is random.

Source:
Purple Book, p. 61

beam current

in in situ microanalysis

The number of primary electrons reaching the surface of the specimen per unit time expressed as electrical current. Recommended symbol: i_{B}; unit: A; typical range: nA. Recommended measurement technique: Faraday cage.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2026

beam diameter

in in situ microanalysis

Diameter of the beam between which 68% of the electrons fall. For Gaussian beam shapes this corresponds to the 2σ-value of the intensity distribution of the beam. Measurement can be carried out by scanning a beam across a sufficiently sharp edge and recording the transmitted electrons.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2027

becquerel

SI derived unit of radioactivity equal to one disintegration per second; admitted for reasons of safeguarding human health, symbol: Bq.

Source:
Green Book, 2nd ed., p. 72
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 963

bed volume

in chromatography

Synonymous with column volume for a packed column.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 832
Orange Book, p. 100

Beer–Lambert law (or Beer–Lambert–Bouguer law)

The absorbance of a beam of collimated monochromatic radiation in a homogeneous isotropic medium is proportional to the absorption path length, l, and to the concentration, c, or — in the gas phase — to the pressure of the absorbing species. The law can be expressed as:

$$A = \log_{10}\left(\frac{P_\lambda^0}{P_\lambda}\right) = \varepsilon\, c\, l$$

or

$$P_\lambda = P_\lambda^0\, 10^{-\varepsilon\, c\, l}$$

where the proportionality constant, ε, is called the molar (decadic) absorption coefficient. For l in cm and c in $\mathrm{mol\ dm^{-3}}$ or M, ε will result in $\mathrm{dm^3\ mol^{-1}\ cm^{-1}}$ or $\mathrm{M\ cm^{-1}}$, which is a commonly used unit. The SI unit of ε is $\mathrm{m^2\ mol^{-1}}$. Note that spectral radiant power must be used because the Beer–Lambert law holds only if the spectral bandwidth of the light is narrow compared to spectral linewidths in the spectrum.
See: absorbance, extinction coefficient, Lambert law

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2230

See also:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1452
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

before mass analysis

in mass spectrometry

The sum of all the separate ion currents for ions of the same sign (usually positive) before mass analysis.

Source:
Orange Book, p. 206

Bell–Evans–Polanyi principle

The linear relation between energy of activation (E_a) and enthalpy of reaction (ΔH_r) sometimes observed within a series of closely related reactions.

$$E_a = A + B\,\Delta H_r$$

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1088

benchmark dose (BMD) and lower effective dose (LED)

The statistical lower bound on a dose corresponding to a specified level of risk.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1021

bending of energy bands

Also contains definition of: flat bands

The distribution of potential in the space charge region of a semiconductor results in a change in the electron energy levels with distance from the interface. This is usually described as 'bending of the energy bands'. Thus the bands are bent, upwards if $\sigma > 0$ and downwards if $\sigma < 0$, where σ is the free charge density. When $\sigma = 0$ the condition of flat bands is met, provided no surface states are present.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 443

Bent's rule

In a molecule, smaller bond angles are formed between electronegative ligands since the central atom, to which the ligands are attached, tends to direct bonding hybrid orbitals of greater *p* character towards its more electronegative substituents.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1926

benzenium ions

Arenium ions, derived from benzene or substituted derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322

benzenonium ions [obsolete]

Obsolescent name for benzenium ions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322

benzylic groups

Arylmethyl groups and derivatives formed by substitution: $ArCR_2$–, Benzyl, $C_6H_5CH_2$–, is the prototype. The term 'benzylic position' or 'benzylic site' refers to the saturated carbon atom. A group, such as –OH, attached at a benzylic site is sometimes referred to as 'benzylic'.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322

benzylic intermediates

Carbanions, carbenium ions or radicals, derived formally by detachment of one hydron, hydride or hydrogen, respectively, from the CH_3 group of toluene or substitution derivatives thereof, e.g. $C_6H_5CH_2^{\cdot}$, benzyl radical.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322

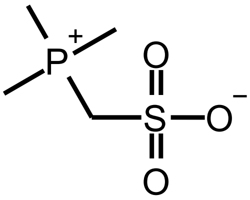
benzynes

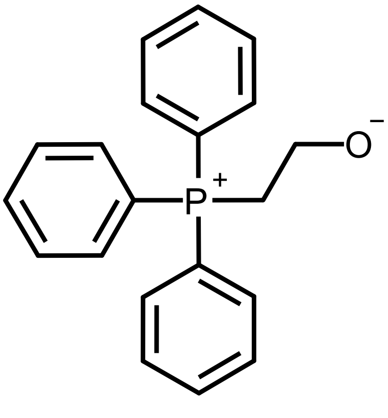
1,2-Didehydrobenzene (the aryne derived from benzene) and its derivatives formed by substitution; see arynes, dehydroarenes. The terms *m*- and *p*-benzyne are occasionally, but erroneously, used for 1,3- and 1,4-didehydrobenzene, respectively.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1088

betaines

Originally, the compound betaine, $(CH_3)_3N^+{-}CH_2C(=O)O^-$ *N,N,N*-trimethylammonioacetate, and similar zwitterionic compounds derived from other amino acids. By extension, neutral molecules having charge-separated forms with an onium atom which bears no hydrogen atoms and that is not adjacent to the anionic atom. Betaines cannot be represented without formal charges. E.g.



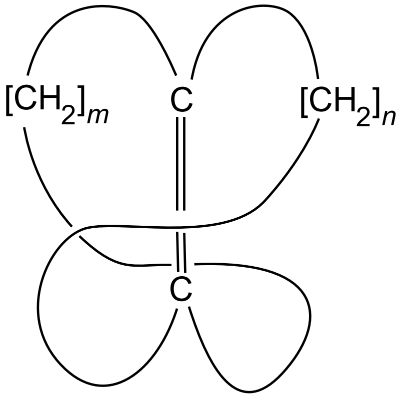


See also: dipolar compounds, mesoionic compounds, ylides, zwitterionic compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322

betweenanenes

Bicyclic alkenes having a double bond between the bridgehead atoms and a *trans* attachment of each branch to the double bond. Thus *trans*-bicyclo[*m*.*n*.0]alk-1 (*m*+2)-enes.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322

bias error

See: measurement result

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1705

biased linear pulse amplifier

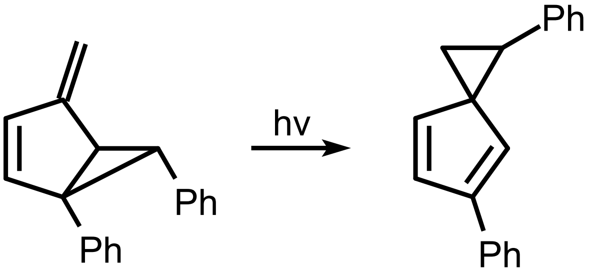
A pulse amplifier which, within the limits of its normal operating characteristics, has a constant gain for that portion of an input pulse that exceeds the threshold value and that produces no output for pulses whose amplitude is below the threshold.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

bicycle rearrangement

Photochemical rearrangement of unsaturated substrates by group migration over a π perimeter following the movement of a bicycle pedal.

An example is:

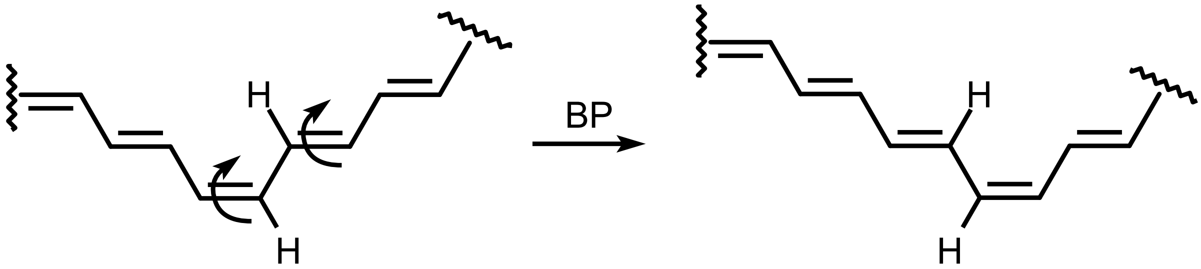


See also: photoisomerization

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 308

bicycle-pedal (BP) mechanism

Volume-conserving mechanism proposed for the photoisomerization of conjugated double bonds. Two alternating double bonds rotate concertedly with only the two CH units turning in and out of the plane of the molecule.



See also: hula-twist mechanism

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 308

bifunctional catalysis

Catalysis (usually for hydron transfer) by a bifunctional chemical species involving a mechanism in which both functional groups are implicated in the rate-controlling step, so that the corresponding catalytic coefficient is larger than that expected for catalysis by chemical species containing only one of these functional groups. The term should not be used to describe the concerted action of two different catalysts ('concerted catalysis').

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1089

bilayer

See: multilayer, monolayer

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1672

bimodal distribution

The occurrence of two maxima in a frequency distribution.

Source:
PAC, 1990, *62*, 17 *(Free energies of cation-molecule complex formation and cation-solvent transfers)* on page 21

bimodal network

Also contains definition of: bimodal polymer network

Polymer network comprising polymer chains having two significantly different molar-mass distributions between adjacent junction points.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1813

binder

Usually a coal tar pitch or petroleum pitch (but may include thermosetting resins or mesophase pitch powders) which, when mixed with a binder coke or a filler, constitutes a carbon mix. This is used in preparation of the formation of shaped green bodies and subsequently carbon artifacts.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 477

binder coke

A constituent of a carbon (or ceramic) artifact resulting from carbonization of the binder during baking.
Note:
Pitches are mainly used as binders, i.e. as precursors for binder cokes, but the term binder should include any carbonaceous binder material, for example thermosetting resins such as poly(furfuryl alcohol) or phenolics and similar compounds which may form a char during carbonization.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 478

binder

in chromatography

An additive used to hold the solid stationary phase to the inactive plate or sheet in thin-layer chromatography.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 830

binding energy

The difference between the total energy of a molecular system and the sum of the energies of its isolated π- and σ-bonds. The value of binding energy depends upon the geometrical arrangement of the isolated subunits (molecules). According to another definition, the term to be subtracted from the total energy is the sum of the energies of the separate atoms in the corresponding valence states, which compose the molecule.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1926

binding site

A specific region (or atom) in a molecular entity that is capable of entering into a stabilizing interaction with another molecular entity. An example of such an interaction is that of an active site in an enzyme with its substrate. Typical forms of interaction are by hydrogen bonding, coordination and ion pair formation. Two binding sites in different molecular entities are said to be complementary if their interaction is stabilizing.

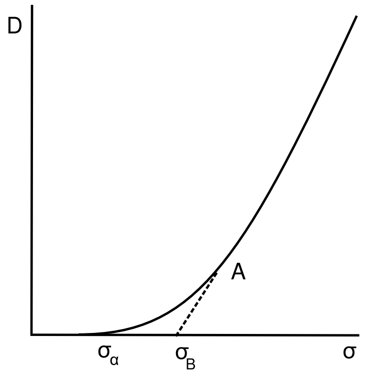
Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1089

Bingham flow

Many colloidal dispersions show Bingham flow which is characterized by a σ-D diagram as shown. At rates of shear greater than that at point A, the following relation applies:

$$\sigma - \sigma_{\mathrm{B}} = \eta_{\Delta}\, D$$

where σ_{B} (or τ_{B}) is called the Bingham yield stress, η_{Δ} is the differential viscosity, D is the shear rate, and σ is the average of three normal stress components if the deformation is purely dilatational.



Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

bioassay

A procedure for determining the concentration or biological activity of a substance (e.g. vitamin, hormone, plant growth factor, antibiotic) by measuring its effect on an organism or tissue compared to a standard preparation.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 147

bioavailability (general)

Extent of absorption of a substance by a living organism compared to a standard system.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1040

bioavailabilty

in pharmacokinetics

Ratio of the systemic exposure from extravascular (ev) exposure to that following intravenous (iv) exposure as described by the equation:

$$F = \frac{A_{\mathrm{ev}}\, D_{\mathrm{iv}}}{B_{\mathrm{iv}}\, D_{\mathrm{ev}}}$$

where F is the bioavailabilty, A and B are areas under the (plasma) concentration-time curve following extravascular and intravenous administration, respectively, and D_{ev} and D_{iv} are the administered extravascular and intravenous doses.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1041

biocatalyst

An enzyme or enzyme complex consisting of, or derived from, an organism or cell culture (in cell-free or whole-cell forms) that catalyses metabolic reactions in living organisms and/or substrate conversions in various chemical reactions.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 147

biochemical (biological) oxygen demand (BOD)

The amount of oxygen, divided by the volume of the system, taken up through the respiratory activity of microorganisms growing on the organic compounds present in the sample (e.g. water or sludge) when incubated at a specified temperature (usually $20\ °\text{C}$) for a fixed period (usually $5\ \text{days}, \text{BOD}_5$). It is a measure of that organic pollution of water which can be degraded biologically. In practice, it is usually expressed in milligrams O_2 per litre.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

biochip

An integrated circuit whose electrical and logical functions are performed by protein molecules appropriately manipulated.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

bioconjugate

A molecular species produced by living systems of biological origin when it is composed of two parts of different origins, e.g. a conjugate of a xenobiotic with some groups, e.g. glutathione, sulfate or glucuronic acid, to make it soluble in water or compartmentalized within the cell.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1260

biodegradable polymer

Polymer susceptible to degradation by biological activity, with the degradation accompanied by a lowering of its molar mass.
Notes:

1. See also Note 2 to polymer degradation.
2. In the case of a polymer, its biodegradation proceeds not only by catalytic activity of enzymes, but also by a wide variety of biological activities.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 898

biodegradation

Breakdown of a substance catalysed by enzymes *in vitro* or *in vivo*. This may be characterized for purposes of hazard assessment as:

1. Primary. Alteration of the chemical structure of a substance resulting in loss of a specific property of that substance.
2. Environmentally acceptable. Biodegradation to such an extent as to remove undesirable properties of the compound. This often corresponds to primary biodegradation but it depends on the circumstances under which the products are discharged into the environment.
3. Ultimate. Complete breakdown of a compound to either fully oxidized or reduced simple molecules (such as carbon dioxide/methane, nitrate/ammonium and water. It should be noted that the products of biodegradation can be more harmful than the substance degraded.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2020
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

bioelectronics

The application of biomolecular principles to microelectronics such as in biosensors and biochips

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

bioisostere

A compound resulting from the exchange of an atom or group of atoms with another, broadly similar, atom or group of atoms.

Source:
PAC, 1998, *70*, 1129 *(Glossary of terms used in medicinal chemistry (IUPAC Recommendations 1998))* on page 1129

biological effect monitoring

Continuous or repeated measurement of early biological effects of exposure to a substance to evaluate ambient exposure and health risk by comparison with appropriate reference values based on knowledge of the probable relationship between ambient exposure and biological effects.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1021

biological exposure index (BEI)

Reference values intended as guidelines for the evaluation of potential health hazards in the practice of industrial hygiene. BEIs represent the levels of determinants that are most likely to be observed in specimens collected from a healthy worker who has been exposed to chemicals to the same extent as a worker with inhalation exposure to the TLV.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1021

biological half life

For a substance the time required for the amount of that substance in a biological system to be reduced to one half of its value by biological processes, when the rate of removal is approximately exponential.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

biological monitoring

Continuous or repeated measurement of potentially toxic substances or their metabolites in tissues, secreta, excreta, expired air, or any combination of these to evaluate occupational or environmental exposure and health risk by comparison with appropriate reference values based on knowledge of the probable relationship between ambient exposure and resultant health effects. Sometimes also called 'biomonitoring'.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1021

biological tolerance values for working materials (Biologische Arbeitsstoff Toleranz Werte (BAT))

The maximum permissible quantity of a chemical compound or its metabolites, or any deviation from the norm of biological parameters induced by those substances in exposed humans.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1022

bioluminescence

Luminescence produced by living systems.
See: luminescence

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2230

biomarker

A parameter that can be used to identify a toxic effect in an individual organism and can be used in extrapolation between species, or as an indicator signalling an event or condition in a biological system or sample and giving a measure of exposure, effect, or susceptibility. The term 'biomarker' is generally used in scientific publications. In occupational hygiene and health, 'biological monitoring' and 'biological effect monitoring' are used with the meaning 'monitoring biomarkers'.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1022
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1042

biomass

Material produced by the growth of microorganisms, plants or animals.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

biomimetic

Refers to a laboratory procedure designed to imitate a natural chemical process. Also refers to a compound that mimics a biological material in its structure or function.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1260

biopolymers

Macromolecules (including proteins, nucleic acids and polysaccharides) formed by living organisms.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

bioreactor

An apparatus used to carry out any kind of bioprocess; examples include fermenter or enzyme reactor.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

biosensor

A device that uses specific biochemical reactions mediated by isolated enzymes, immunosystems, tissues, organelles or whole cells to detect chemical compounds usually by electrical, thermal or optical signals.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

biosphere

in atmospheric chemistry

That part of the globe that encompasses all forms of life on the earth. It extends from the ocean depths to a few thousand metres of altitude in the atmosphere, and includes life forms at the earth's surface, in soils and constituents which exchange materials with atmospheres, oceans or surfaces.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

biosynthesis

The production of a chemical compound by a living organism (cf. biotransformation).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

biotechnology

The integration of natural sciences and engineering sciences in order to achieve the application of organisms, cells, parts thereof and molecular analogues for products and services.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

biotransformation

Synonym: bioconversion

Any chemical conversion of substances that is mediated by living organisms or enzyme preparations derived therefrom.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

biphotonic excitation

Simultaneous (coherent) absorption of two photons (either same or different wavelength), the energy of excitation being the sum of the energies of the two photons. Also called two-photon excitation.
Note:
This term is sometimes also used for a two-step absorption.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 308

biphotonic process

Resulting from biphotonic excitation.
See: multiphoton process

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 308

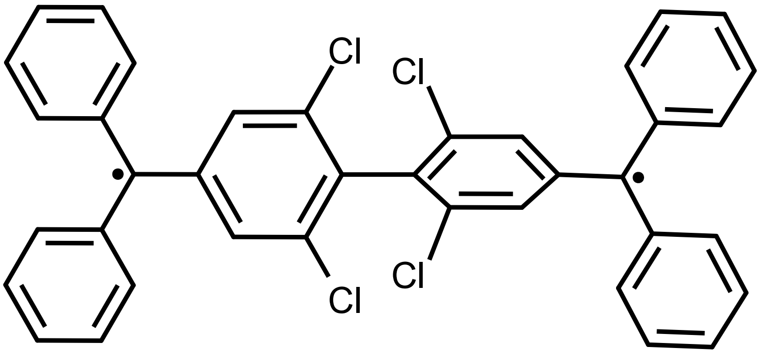
bipolarons

Bound pairs of polarons mutually attracted by the lattice distortion in a solid.
See also: self-localized excitations.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 309

biradical

An even-electron molecular entity with two (possibly delocalized) radical centres which act nearly independently of each other, e.g.

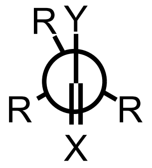


Species in which the two radical centres interact significantly are often referred to as 'biradicaloids'. If the two radical centres are located on the same atom, the species are more properly referred to by their generic names: carbenes, nitrenes, etc. The lowest-energy triplet state of a biradical lies below or at most only a little above its lowest singlet state (usually judged relative to $k_B\ T$, the product of the Boltzmann constant k_B and the absolute temperature T). The states of those biradicals whose radical centres interact particularly weakly are most easily understood in terms of a pair of local doublets. Theoretical descriptions of low-energy states of biradicals display the presence of two unsaturated valences (biradicals contain one fewer bond than permitted by the rules of valence): the dominant valence bond structures have two dots, the low energy molecular orbital configurations have only two electrons in two approximately nonbonding molecular orbitals, two of the natural orbitals have occupancies close to one, etc. Although this term has been recommended in the past for diradicals, specialists working in the field prefer the latter term.
See also: carbenes, nitrenes

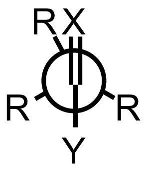
Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1089
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322

bisecting conformation (eclipsing conformation)

For a structure containing the grouping $R_3C–C(Y)=X$ (with identical or different groups R) the conformation in which the torsion angle is such that X is antiperiplanar to one of the groups R , and, in a Newman projection, the double bond C=X bisects one of the R–C–R angles. In this conformation the bond C–Y eclipses one of the C–R bonds. The other conformation, in which X is synperiplanar to one of the groups R , is called an eclipsing conformation.



bisecting conformation



eclipsing conformation

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2201

bismuthanes

The saturated hydrides of tervalent bismuth, having the general formula Bi_nH_{n+2} . Hydrocarbyl derivatives of BiH_3 belong to the class bismuthines.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1322

bismuthines

BiH_3 and compounds derived from it by substituting one, two or three hydrogen atoms by hydrocarbyl groups: R_3Bi, $RBiH_2$, R_2BiH ($R \neq H$) are called primary, secondary and tertiary bismuthines, respectively. A specific bismuthine is preferably named as a substituted bismuthane, e.g. $(CH_3)_3Bi$ trimethylbismuthane.
See: bismuthanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

bisphenols

By usage, the methylenediphenols, $HOC_6H_4CH_2C_6H_4OH$, commonly *p,p*-methylenediphenol, and their substitution products (generally derived from condensation of two equivalent amounts of a phenol with an aldehyde or ketone).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

bivane

in atmospheric chemistry

A wind vane used in turbulence studies to obtain horizontal and vertical components of the wind vector.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

black film

Also contains definition of: common black film

A film thinner than about $\frac{1}{4}$ wavelength of visible light. Black films are often equilibrium films, but equilibrium films may be considerably thicker under some conditions. In soap films, two types of equilibrium film are often observed: the one characterized by thickness of the order of $7\ \mathrm{nm}$ or more which varies significantly with minor changes in composition such as ionic strength, is called common black film.
See also: Newton black film

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 614

blank value

in analysis

A reading or result originating from the matrix, reagents and any residual bias in the measurement device or process, which contributes to the value obtained for the quantity in the analytical procedure.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1662
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

blaze-angle

in spectrochemical analysis

The angle (β) between the operating facet of the grooves and the overall plane of a grating.

Source:
Orange Book, p. 157

bleaching

in photochemistry

The loss of absorption or emission intensity.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2231

block

A portion of a macromolecule, comprising many constitutional units that has at least one feature which is not present in the adjacent portions. Where appropriate, definitions relating to 'macromolecule' may also be applied to 'block'.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2298

block copolymer

A copolymer that is a block polymer. In the constituent macromolecules of a block copolymer, adjacent blocks are constitutionally different, i.e. adjacent blocks comprise constitutional units derived from different species of monomer or from the same species of monomer but with a different composition or sequence distribution of constitutional units.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2303

block macromolecule

A macromolecule which is composed of blocks in linear sequence.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2292

block polymer

A polymer composed of block macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2303

blotting

in biotechnology

A technique used for transferring DNA, RNA or protein from gels to a suitable binding matrix, such as nitrocellulose or Nylon paper, while maintaining the same physical separation.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 148

blowdown

in atmospheric chemistry

Hydrocarbons purged during refinery shutdowns and startups which should be piped to storage systems for safe venting, flaring or recovery. This term also applies to the purging of water in boiler operation, and serves in the control of dissolved solids in the boiler water.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

blue shift

Informal expression for hypsochromic shift.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2231

boat

See: chair, boat, twist, half-chair

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2201

Bodenstein approximation

See: steady state

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1089

body burden

Total amount of substance of a chemical present in an organism at a given time.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1022

bohr

Atomic unit of length,

$$a_0 \approx 5.291\,772\,49(24) \times 10^{-11}\ \mathrm{m}.$$

Source:
Green Book, 2nd ed., p. 76

Bohr magneton

Electromagnetic fundamental physical constant:

$$\mu_\mathrm{B} = \frac{e\,\hbar}{2\,m_\mathrm{e}} = 9.274\,0154\ (31) \times 10^{-24}\ \mathrm{J\,T^{-1}}$$

where e is the elementary charge, $\hbar$ the Planck constant divided by $2\,\pi$ and m_e the electron rest mass.

Source:
CODATA Bull. 1986, *63*, 1

Bohr radius

Atomic fundamental physical constant used as atomic unit of length:

$$a_0 = \frac{4\,\pi\,\varepsilon_0\,\hbar^2}{m_\mathrm{e}\,e^2} = 5.291\,772\,49\ (24) \times 10^{-11}\ \mathrm{m}$$

where e the elementary charge, $\hbar$ the Planck constant divided by $2\,\pi$ and m_e the electron rest mass.

Source:
CODATA Bull. 1986, *63*, 1

bolometer

A detector constructed from a material having a large temperature coefficient of resistance. Absorption of radiation gives rise to a change in resistance. A bolometer is named according to its active component, e.g. thermistor bolometer, semiconductor bolometer, superconductor bolometer.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1752

Boltzmann constant

Fundamental physical constant: $k = \frac{R}{L} = 1.380\,6504\ (24) \times 10^{-23}\ \mathrm{J\ K^{-1}}$, where R is the gas constant and L the Avogadro constant.

Source:
CODATA 2006
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 963

bomb-digestion

in spectrochemical analysis

Materials which are not fully dissolved by acid-digestion at atmospheric pressure may require a more vigorous treatment in pressure vessels lined with polytetrafluoroethylene (PTFE) glass, silica or vitreous (glassy) carbon or in sealed silica tubes; this treatment is called bomb-digestion. The test sample and acids are heated in such a closed vessel, so that the digestion is carried out at higher temperature and pressure.

Source:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1469

bond

There is a chemical bond between two atoms or groups of atoms in the case that the forces acting between them are such as to lead to the formation of an aggregate with sufficient stability to make it convenient for the chemist to consider it as an independent 'molecular species'.
See also: agostic, coordination, hydrogen bond, multi-centre bond

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1089

bond dissociation

See: heterolysis, homolysis
(In ordinary usage the term refers to homolysis only.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1089

bond energy

in theoretical chemistry

The energy required to break a given type of bond between atoms in certain valence states. An averaged bond energy is commonly derived by dissecting the heat of atomization of a molecule into contributions of individual bonds. For molecules with localized bonds, the heats of atomization (formation) are usually well approximated by the sum of pertinent averaged bond energies.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1927

bond energy (mean bond energy)

The average value of the gas-phase bond dissociation energies (usually at a temperature of $298\ \mathrm{K}$) for all bonds of the same type within the same chemical species. The mean bond energy for methane, for example, is one-fourth the enthalpy of reaction for:

$$\mathrm{CH_4(g)} \longrightarrow \mathrm{C(g)} + 4\,\mathrm{H(g)}$$

Tabulated bond energies are generally values of bond energies averaged over a number of selected typical chemical species containing that type of bond.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1090

bond length

The distance between atomic centers involved in a chemical bond. The notion of bond length is defined differently in various experimental methods of determination of molecular geometry; this leads to small (usually $0.01 - 0.02\ \text{Å}$) differences in bond lengths obtained by different techniques. For example, in gas-phase electron-diffraction experiments, the bond length is the interatomic distance averaged over all occupied vibrational states at a given temperature. In an X-ray crystal structural method, the bond length is associated with the distance between the centroids of electron densities around the nuclei. In gas-phase microwave spectroscopy, the bond length is an effective interatomic distance derived from measurements on a number of isotopic molecules, etc. A number of empirical relationships between bond lengths and bond orders in polyatomic molecules were suggested, see, for example, fractional bond number (the Pauling's bond order).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1927

bond number

The number of electron-pair bonds between two nuclei in any given Lewis formula. For example, in ethene the bond number between the carbon atoms is two, and between the carbon and hydrogen atoms it is one.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1090

bond orbital

A localized molecular orbital related to a certain σ-, π-, or δ-bond.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1927

bond order

The electron population in the region between atoms A and B of a molecular entity at the expense of electron density in the immediate vicinity of the individual atomic centers. Different schemes of partitioning electron density give rise to different definitions of bond orders. In the framework of the Mulliken population analysis, bond order is associated with the total overlap population

$$q_{AB} = 2 \sum_{\mu}^{A} \sum_{\nu}^{B} P_{\mu\nu} S_{\mu\nu}$$

where $P_{\mu\nu}$ and $S_{\mu\nu}$ are respectively the elements of the density matrix and overlap matrix (see overlap integral). A large positive value of bond order signifies strong bonding between the atoms of the molecular entity, whereas negative values of q_{AB} imply that electrons are displaced away from the inter-atomic region and point to an anti-bonding interaction. In valence bond theory, bond order is given by a weighted average of the formal bond orders (i.e. by the number of electron pairs in a given Lewis structure) between the atoms in the resonance structures (see resonance hybrid).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1927

bond order p_{rs}

Theoretical index of the degree of bonding between two atoms relative to that of a single bond, i.e. the bond provided by one localized electron pair. In molecular orbital theory it is the sum of the products of the corresponding atomic orbital coefficients (weights) over all the occupied molecular spin-orbitals.

Source:
Green Book, 2nd ed., p. 17

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1090

bond-dissociation energy, *D*

The enthalpy (per mole) required to break a given bond of some specific molecular entity by homolysis, e.g. for $CH_4 \longrightarrow {}^{\bullet}CH_3 + H^{\bullet}$, symbolized as $D(CH_3{-}H)$ (cf. heterolytic bond dissociation energy).
See also: bond energy

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1089
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

bond-dissociation energy (BDE)

in theoretical chemistry

For a diatomic molecule, the maximum vibrational energy that a molecule can have prior to its decomposition into the ground electronic states of the constituent atoms (spectroscopic bond-dissociation energy, D_e). The D_e value is related to the chemical dissociation energy: $D_0 = D_e - E_{vib}(0)$, where $E_{vib}(0)$ is zero-point vibrational energy. This definition is usually extended to the dissociation of polyatomic molecules into certain molecular fragments through homolytic or heterolytic bond cleavages.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1928

bond-energy-bond-order method

An empirical procedure for estimating activation energies, involving empirical relationships between bond length, bond dissociation energy, and bond order.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 154

bonded phase

in chromatography

A stationary phase which is covalently bonded to the support particles or to the inside wall of the column tubing.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 823

bonding molecular orbital

The molecular orbital whose occupation by electrons increases the total bonding (usually, lowers the total energy) of a molecule. Generally, the energy level of a bonding MO lies lower than the average of the valence orbitals of the atoms constituting the molecule.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1929

bonding number

The bonding number n of a skeletal atom is the sum of the total number of bonding equivalents (valence bonds) of that skeletal atom to adjacent skeletal atoms in a parent hydride, if any, and the number of attached hydrogen atoms, if any. Examples: SH_2: for S, $n = 2$; SH_6: for S, $n = 6$.

Source:
Blue Book (Guide), p. 21

See also:
PAC, 1984, *56*, 769 *(Treatment of variable valence in organic nomenclature (lambda convention) (Recommendations 1983))* on page 774

boranes

The molecular hydrides of boron, e.g. B_5H_9 pentaborane(9).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

boranylidenes

The species RB: containing an electrically neutral univalent boron atom with two formally non-bonding electrons.
See: carbene analogues

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

borderline mechanism

A mechanism intermediate between two extremes, for example a nucleophilic substitution intermediate between S_N1 and S_N2, or intermediate between electron transfer and S_N2.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1090

borenes

A traditional term for boranylidenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

borinic acids

Compounds having the structure R_2BOH.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

Born–Oppenheimer (BO) approximation

Representation of the complete wavefunction as a product of an electronic and a nuclear part

$$\Psi(\mathrm{r},\mathrm{R}) = \Psi_{\mathrm{e}}(\mathrm{r},\mathrm{R})\,\Psi_{\mathrm{N}}(\mathrm{R})$$

where the two wave-functions may be determined separately by solving two different Schroedinger equations. The validity of the Born–Oppenheimer approximation is founded on the fact that the ratio of electronic to nuclear mass ($\frac{m}{M} \cong 5 \times 10^{-4}$) is sufficiently small and the nuclei, as compared to the rapidly moving electrons, appear to be fixed. The approximation breaks down near a point where two electronic states acquire the same energy (see Jahn–Teller effect). The BO approximation is often considered as being synonymous with the adiabatic approximation. More precisely, the latter term denotes the case when Ψ_{e} diagonalize the electronic Hamiltonian. Thus, the adiabatic approximation is an application of the BO approximation.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1929

boronic acids

Compounds having the structure $RB(OH)_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

borylenes

A traditional term for boranylidenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

boson

Particle of integer spin quantum number following Bose–Einstein statistics.

Source:
Physical Chemistry Division, unpublished

bound fraction

in radioanalytical chemistry

The fraction of the incubation mixture which, after separation, contains the analyte bound to the binding reagent.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2519

boundary layer

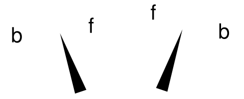
in atmospheric chemistry

That well-mixed region of the lower atmosphere in which the turbulence is maintained largely by convective buoyancy induced by the upward heat flux originating from the solar-heated surface of the earth. During the afternoon this often extends from $1\ \mathrm{km}$ to $5\ \mathrm{km}$ in height. The surface boundary layer is that region of the lower atmosphere where the shearing stress is constant. It is separated by the Ekman layer from the free atmosphere, where the behaviour of the atmosphere approaches that of an ideal fluid in approximate geostrophic equilibrium (horizontal coriolis force balances the horizontal pressure force at all points in the field).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

bowsprit (flagpole)

In the boat form of cyclohexane and related structures there are two ring atoms lying out of the plane of the other four; exocyclic bonds to these two atoms pointing in a direction roughly parallel to that plane are called bowsprit, the other two are called flagpole.



b = bowsprit
f = flagpole

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2201

branch point

in polymers

Point on a polymer chain at which a branch is attached.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1818

branch (side chain, pendant chain)

Also contains definitions of: long-chain branch, short-chain branch

in polymers

An oligomeric or polymeric offshoot from a macromolecular chain.
Notes:

1. An oligomeric branch may be termed a short-chain branch.
2. A polymeric branch may be termed a long-chain branch.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2297

branch unit

Also contains definition of: *f*-functional branch unit

in polymers

A constitutional unit containing a branch point.
Note:
A branch unit from which f linear chains emanate may be termed an f-functional branch unit, e.g. five-functional branch unit. Alternatively, the terms trifunctional, tetrafunctional, pentafunctional, etc. may be used, e.g. pentafunctional branch unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2297

branched chain

in polymers

A chain with at least one branch point intermediate between the boundary units.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2293

branched polymer

in polymers

A polymer the molecules of which are branched chains.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2304

branching chain reaction

A chain reaction which includes a propagation step or steps in which there is an increase in the number of active intermediates; for example,

$$\mathrm{H} + \mathrm{O_2} \longrightarrow \mathrm{OH} + \mathrm{O}$$

is a branching reaction since one active intermediate (H) gives rise to two (OH and O).

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 762

branching decay

Nuclear decay which can proceed in two or more different ways.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

branching fraction

In branching decay the fraction of nuclei which decay in a specified way.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

branching index

in polymers

A parameter, g, characterizing the effect of long-chain branches on the size of a branched macromolecule in solution and defined as the ratio of the mean-square radius of gyration of a branched molecule, $< s_{\mathrm{b}}^2 >$, to that of an otherwise identical linear molecule, $< s_{\mathrm{l}}^2 >$, with the same relative molecular mass in the same solvent and at the same temperature, i.e. $g = \frac{< s_{\mathrm{b}}^2 >}{< s_{\mathrm{l}}^2 >}$.

Source:
Purple Book, p. 51

branching plane

At a conical intersection point, the plane spanned by the gradient difference vector ($\boldsymbol{x}_1$) and the gradient of the interstate coupling vector ($\boldsymbol{x}_2$):

$$\boldsymbol{x}_1 = \frac{\partial(E_2 - E_1)}{\partial Q}\,\boldsymbol{q}$$

$$\boldsymbol{x}_2 = \, < \boldsymbol{C}_1^t \left(\frac{\partial H}{\partial Q}\right) \boldsymbol{C}_2 > \, \boldsymbol{q}$$

where $\boldsymbol{C}_1$ and $\boldsymbol{C}_2$ are the configuration interaction eigenvectors (i.e., the excited and ground-state adiabatic wavefunctions) in a conical intersection problem, H is the conical intersection Hamiltonian, $\boldsymbol{Q}$ represents the nuclear configuration vector of the system, and thus $\boldsymbol{q}$ is a unit vector in the direction of vector $\boldsymbol{q}$. E_1 and E_2 are the energies of the lower and upper states, respectively.
Note:
The branching plane is also referred to as the ***g*-*h*** plane. Inspection of $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ provides information on the geometrical deformation imposed on an excited state molecular entity immediately after decay at a conical intersection. Consequently, these vectors provide information on the ground-state species that will be formed after the decay.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 309

branching ratio

The ratio of alternative products formed in a reaction (e.g. the HF / DF ratio in the reaction between F and HD).

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 154
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1536

break

of a foam

The process involving the coalescence of gas bubbles.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 611

break

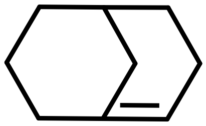
of an emulsion

The flocculation of an emulsion, viz. the formation of aggregates may be followed by coalescence. If coalescence is extensive it leads to the formation of a macrophase and the emulsion is said to break.

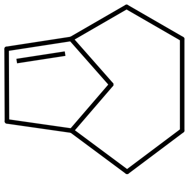
Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 611

Bredt's rule

A double bond cannot be placed with one terminus at the bridgehead of a bridged ring system unless the rings are large enough to accommodate the double bond without excessive strain. For example, while bicyclo[2.2.1]hept-1-ene is only capable of existence as a transient, its higher homologues having a double bond at the bridgehead position have been isolated: e.g.



bicyclo[3.3.1]non-1-ene



bicyclo[4.2.1]non-1(8)-ene

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1077

See also:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2201

breeching

in atmospheric chemistry

The passage or conduit through which the exhaust products of combustion are carried to the stack or chimney.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2176

breeze

in atmospheric chemistry

A term sometimes used to describe very fine particles of coke. Also a meteorological term for a gentle wind.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2177

Bremsstrahlung

X-radiation emitted as a result of the retardation of high energy particles by matter.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 737

Brewster angle, θ_B

When an unpolarized planar electromagnetic wavefront impinges on a flat dielectric surface, there is a unique angle (θ_B), commonly referred to as Brewster angle, at which the reflected waves are all polarized into a single plane.
Notes:

1. Expression for Brewster angle:

$$\theta_\mathrm{B} = \arctan \frac{n_2}{n_1} = \arctan \left(\frac{\varepsilon_2}{\varepsilon_1}\right)^{1/2}$$

   where n_2 and n_1 are the refractive indices of the receiving surface and the initial medium, respectively, and ε_2 and ε_1 are the relative static permittivities (formerly called dielectric constants).
2. For a randomly polarized beam incident at Brewster angle, the electric fields of the reflected and refracted waves are perpendicular to each other
3. For a wave incident from air on water ($n = 1.333$), glass ($n = 1.515$), and diamond ($n = 2.417$), the Brewster angles are 53, 57, and $67.5\ \mathrm{degrees}$, respectively.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 310

bridge

Also contains definition of: bridgehead

A valence bond or an atom or an unbranched chain of atoms connecting two different parts of a molecule. The two tertiary carbon atoms connected through the bridge are termed bridgeheads.

Source:
Blue Book, p. 31

bridge index

In a coordination entity, the number of central atoms linked by a particular bridging ligand.

Source:
Red Book, p. 149

bridge solution

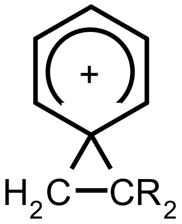
in pH *measurement*

Solution of high concentration of inert salt, preferably comprising cations and anions of equal mobility, optionally interposed between the reference electrode filling and both the test and standard solution, when the test solution and filling solution are chemically incompatible. This procedure introduces into the operational cell a second liquid junction formed usually in a similar way to the first. (This definition refers to a bridge solution of a double junction reference electrode.)

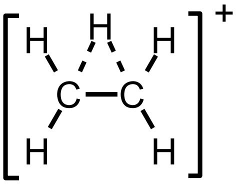
Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 541

bridged carbocation

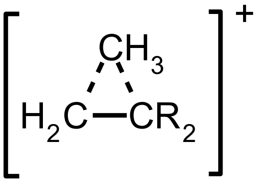
A carbocation (real or hypothetical) in which there are two (or more) carbon atoms that could in alternative Lewis formulae be designated as carbenium centres but which is instead represented by a structure in which a group (a hydrogen atom or a hydrocarbon residue, possibly with substituents in non-involved positions) bridges these potential carbenium centres. One may distinguish 'electron-sufficient bridged carbocations' and 'electron-deficient bridged carbocations'. Examples of the former are phenyl-bridged ions (for which the trivial name 'phenonium ion' has been used), such as (A). These ions are straightforwardly classified as carbenium ions. The latter type of ion necessarily involves three-centre bonding. Structures (C) and (D) contain five-coordinate carbon atoms. The 'hydrogen-bridged carbocation' (B) contains a two-coordinate hydrogen atom. Hypercoordination, which includes two-coordination for hydrogen and five- but also higher coordination for carbon is generally observed in bridged carbocations.



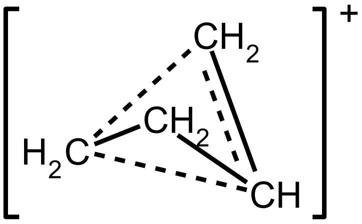
(A)



(B)



(C)



(D)

See also: carbonium ion, multi-centre bond, neighbouring group participation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1090

bridging ligand

A ligand attached to two or more, usually metallic, central atoms.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1091
Red Book, p. 149
Blue Book, p. 338

brightness

Obsolete term. This term is reserved for non-quantitative reference to physiological perception of light and is not recommended as a quantitative measure of the radiance of an emitting device, e.g., a lamp.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 310

brightness

of a laser dye

Product of the fluorescence quantum yield (Φ_f) of a dye and the molar decadic absorption coefficient at the excitation wavelength, $\varepsilon(\lambda)$, i.e., $\Phi_f \, \varepsilon(\lambda)$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 310

bromohydrins

See: halohydrins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

Brooks and Taylor structure

The structure of the anisotropic spheres which precipitate from isotropic pitch during pyrolysis. The structure of the spheres consists of a lamellar arrangement of aromatic molecules in parallel layers which are perpendicular to the polar axis of the sphere and which are perpendicular to the mesophase-isotropic phase interface.
Note:
The term Brooks and Taylor structure is recommended to describe the particular lamellar morphology of the spherules most commonly precipitated from pyrolysed pitch. The term honours the workers who first recognized the significance of carbonaceous mesophase to carbon science and technology and who first defined this spherical morphology. The term Brooks and Taylor structure does not cover all structures found in the spherical mesophase, because other lamellar arrangements have been observed.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 478

Brownian motion

The movement of particles in a colloidal system such as an aerosol caused by collision with the molecules in the fluid in which the particles are imbedded.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2177

Brønsted acid

A molecular entity capable of donating a hydron (proton) to a base, (i.e. a 'hydron donor') or the corresponding chemical species. For example: H_2O, H_3O^+, CH_3CO_2H, H_2SO_4, HSO_4^-, HCl, CH_3OH, NH_3 .
See also: conjugate acid–base pair

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1091

Brønsted base

A molecular entity capable of accepting a hydron (proton) from an acid (i.e. a 'hydron acceptor') or the corresponding chemical species. For example: OH^-, H_2O, $CH_3CO_2^-$, HSO_4^-, SO_4^{2-}, Cl^- .
See also: conjugate acid-base pair

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1091

Brønsted relation

Also contains definition of: catalysis law

The term applies to either of the equations:

$$\frac{k_{\mathrm{HA}}}{p} = G\left(\frac{q\,K_{\mathrm{HA}}}{p}\right)^{\alpha}$$

$$\frac{k_{\mathrm{A}}}{q} = G\left(\frac{q\,K_{\mathrm{HA}}}{p}\right)^{-\beta}$$

(or their logarithmic forms) where α, β and G are constants for a given reaction series (α and β are called 'Brønsted exponents'), k_{HA} and k_{A} are catalytic coefficients (or rate coefficients) of reactions whose rates depend on the concentrations of HA and/or of A^- . K_{HA} is the acid dissociation constant of the acid HA, p is the number of equivalent acidic protons in the acid HA, and q is the number of equivalent basic sites in its conjugate base A^-. The chosen values of p and q should always be specified. (The charge designations of H and A are only illustrative.) The Brønsted relation is often termed the 'Brønsted catalysis law' (or the 'Catalysis Law'). Although justifiable on historical grounds, this name is not recommended, since Brønsted relations are known to apply to many uncatalysed and pseudo-catalysed reactions (such as simple proton (hydron) transfer reactions). The term 'pseudo-Brønsted relation' is sometimes used for reactions which involve nucleophilic catalysis instead of acid–base catalysis. Various types of Brønsted parameters have been proposed such as β_{lg}, β_{nuc}, β_{eq} for leaving group, nucleophile and equilibrium constants, respectively.
See also: linear free–energy relation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1091
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 154

bubble column

A bioreactor, in the shape of a column, in which the reaction medium is kept mixed and aerated by introduction of air into the bottom (cf. air lift bioreactor).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 149

bubbler

in atmospheric chemistry

An apparatus used to absorb certain water soluble components in a gas stream for later analysis. Usually it involves the use of a glass fritted tube which forces the air into small bubbles of high surface area during operation.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2177

buffer-addition technique

in analytical flame spectroscopy

A technique in which an additive (called a spectrochemical buffer) is added to both the sample and reference solutions for the purpose of making the measure of the analyte less sensitive to variations in interferent concentration.

Source:
Orange Book, p. 172

bulk concentration

in electroanalysis

In any technique that involves the establishment of a concentration gradient, either within the material from which an electrode is made or in the solution that is in contact with an electrode, the bulk concentration of a substance **B** is the total or analytical concentration of **B** at points so remote from the electrode-solution interface that the concentration gradient for **B** is indistinguishable from zero at the instant under consideration. In common practice the bulk concentration of **B** is taken to be the total or analytical concentration of **B** that would be present throughout the electrode or solution if there were no current flowing through the cell and if the electrode and solution did not interact in any way. In the absence of any homogeneous reaction or other process that produces or consumes

B, the bulk concentration of **B** is the total or analytical concentration of **B** that is present before the excitation signal is applied.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1493

bulk mesophase

A continuous anisotropic phase formed by coalescence of mesophase spheres. Bulk mesophase retains fluidity and is deformable in the temperature range up to about $770\ \mathrm{K}$, and transforms into green coke by further loss of hydrogen or low-molecular-weight species. This bulk mesophase can sometimes be formed directly from the isotropic pitch without observation of intermediate spheres.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 478

bulk rheology

Also contains definition of: surface rheology

Rheology may be conveniently divided into bulk rheology, in which effects due to the surface of the system can be neglected, and surface rheology, in which such effects are predominant. It should be noted that in surface rheology the neglect of bulk behaviour is permissible only in exceptional circumstances, such as for very thin films surrounded by a gas.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1215

bulk sample

The sample resulting from the planned aggregation or combination of sample units.

Source:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1463

Bunnett–Olsen equations

The equations for the relation between $\log_{10}\left(\frac{[\mathrm{SH}^{+}]}{[\mathrm{S}]}\right) + H_0$ and $\log_{10}[\mathrm{H}^{+}] + H_0$ for base S in aqueous mineral acid solution, where H_0 is Hammett's acidity function and $\log_{10}[\mathrm{H}^{+}] + H_0$ represents the activity function $\frac{\log_{10}(\gamma_S\, \gamma_{H^+})}{\gamma_{\mathrm{SH}^+}}$ for the nitroaniline reference bases to build H_0.

$$\log_{10}\left(\frac{[\mathrm{SH}^+]}{[\mathrm{S}]}\right) - \log_{10}[\mathrm{H}^+] = (\Phi - 1)\,(\log_{10}[\mathrm{H}^+] + H_0) + \mathrm{p}K_{\mathrm{SH}^+}$$

$$\log_{10}\left(\frac{[\mathrm{SH}^+]}{[\mathrm{S}]}\right) + H_0 = \Phi\,(\log_{10}[\mathrm{H}^+] + H_0) + \mathrm{p}K_{\mathrm{SH}^+}$$

See also: Cox–Yates equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1091

Bunsen burner

Also contains definitions of: Meker burner, slot burner

Premix burners are distinguished as Bunsen-, Meker-, or slot-burners according to whether they have one large hole, a number of small holes, or a slot as outlet port(s) for the gas mixture, respectively. When several parallel slots are present, they are identified as multislot burners (e.g. a three-slot burner).

Source:
Orange Book, p. 166

Bunte salts [obsolete]

Salts (usually sodium salts) of *S*-alkylthiosulfuric acid, of general structure $\mathrm{RSS(=O)_2O^-M^+}$. Use of this term is discouraged.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

burn-up

Induced nuclear transformation of atoms during reactor operation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

burn-up fraction

The fraction of an initial quantity of a given nuclide that has undergone burn-up.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

burning tension

of an electrical arc

See: electrical arc

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1464

burning velocity, v_b

of a flame front

in flame emission and absorption spectrometry

The mean velocity of the flame front (in $\mathrm{mm\ s^{-1}}$) towards the unburnt gas mixture (usually vertically downwards). The quantity applies to gas mixtures and not to injection burners, and depends on the flame temperature and the solvent nebulized.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1742

bypass injector

in gas chromatography

A sample injector by means of which the eluent (carrier gas) may be temporarily diverted through a sample chamber so that the sample is carried to the column.

Source:
Orange Book, p. 99

χ-parameter

A numerical parameter, χ, employed in the Flory–Huggins theory, which accounts in the main for the contribution of the non-combinatorial entropy of mixing and for the enthalpy of mixing.

Source:
Purple Book, p. 59

C-terminal residue

in a polypeptide

See: amino-acid residue *in a polypeptide*

Source:
White Book, p. 48

C. I. P. system

Short for Cahn–Ingold–Prelog system.
See: CIP priority

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2201

cage

An aggregate of molecules, generally in the condensed phase, that surrounds the fragments formed, for example, by thermal or photochemical dissociation. Because the cage hinders the separation of the fragments by diffusion, they may preferentially react with one another (' cage effect ') but not necessarily to reform the precursor species. For example:

$$\mathrm{R{-}N{=}N{-}R} \xrightarrow{\Delta} \left[\mathrm{R}^{\bullet} + \mathrm{N{\equiv}N} + {}^{\bullet}\mathrm{R}\right]_{\mathrm{cage}} \longrightarrow \mathrm{R{-}R} + \mathrm{N_2}$$

See: geminate recombination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1091

cage compound

A polycyclic compound having the shape of a cage. The term is also used for inclusion compounds.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1092

cage effect

When in a condensed phase, or in a dense gas, reactant molecules come together, or species are formed in proximity to one another, and are caged in by surrounding molecules, they may undergo a set of collisions known as an encounter; the term 'cage effect' is then applied.
The cage effect is also known as the Franck–Rabinowitch effect.
See also: cage.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 155

Cahn–Ingold–Prelog system

See: CIP priority

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2201

calcination

Heating to high temperatures in air or oxygen.
Notes:
1. The term is most likely to be applied to a step in the preparation of a catalyst.
2. In sol-gel processing the term applies to the heating of a polymer network containing metal compounds to convert it into an oxide network.
3. Modified from previous definition. The definition proposed here is more explicit about the elevated temperatures that are required.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1821

calcined coke

A petroleum coke or coal-derived pitch coke obtained by heat treatment of green coke to about $1600\ \mathrm{K}$. It will normally have a hydrogen content of less than $0.1\ \mathrm{wt.\%}$.
Note:
Calcined coke is the main raw material for the manufacture of polygranular carbon and polygranular graphite products (e.g. carbon and graphite electrodes).

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 479

calibration component

A component of a calibration mixture, present in the gaseous or vapour state, quantitatively and qualitatively defined, and used directly for testing and for calibration.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2177

calibration function
Also contains definition of: calibration curve

in analysis

The functional (not statistical) relationship for the chemical measurement process, relating the expected value of the observed (gross) signal or response variable $E(y)$ to the analyte amount x. The corresponding graphical display for a single analyte is referred to as the calibration curve. When extended to additional variables or analytes which occur in multicomponent analysis, the 'curve' becomes a calibration surface or hypersurface.

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1703

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2177

calibration gas mixture

in atmospheric chemistry

A gas mixture of known composition, generally comprising one or more calibration components and a complementary gas.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2177

calibration

in analysis

The set of operations which establish, under specified conditions, the relationship between values indicated by the analytical instrument and the corresponding known values of an analyte.
See: calibration material

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1662

calibration material

in analysis

A material of known composition or properties which can be presented to the analytical instrument for calibration purposes.
See also: control material

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

calibration mixture

in analysis

A gaseous or liquid mixture of known composition, generally comprising one or more calibration components and an inert diluent, used directly for testing and calibration of analytical instruments.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2178

calibration sample

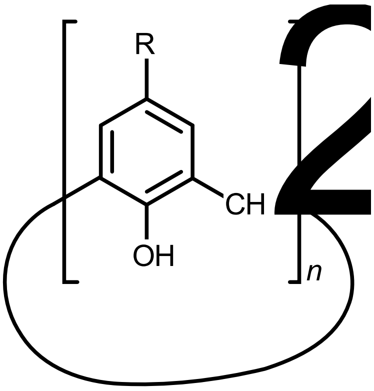
in analysis

The test portion or test solution used for calibration of an analytical procedure. The calibration sample is normally of known weight or volume and is prepared according to specifications.
See also: test portion, test solution, measurement solution

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

calixarenes

Originally macrocyclic compounds capable of assuming a basket (or 'calix') shaped conformation. They are formed from p- hydrocarbyl phenols and formaldehyde. The term now applies to a variety of derivatives by substitution of the hydrocarbon cyclo{oligo[(1,3-phenylene)methylene]}.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

calorie

Non-SI unit of energy. There are three differently defined calories: thermochemical calorie ($\mathrm{cal_{th}} = 4.184\ \mathrm{J}$), international steam table calorie ($\mathrm{cal_{IT}} = 4.1868\ \mathrm{J}$), 15 °C calorie ($\mathrm{cal_{15}} = 4.1855\ \mathrm{J}$), however only the symbol cal is usually used.

Source:
Green Book, 2nd ed., p. 112
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 964

calorimetric titration

A titration performed in a calorimeter which produces a plot of heat change versus volume of titrant. This is the preferred term for experiments in which the main goal is the measurement of thermodynamic parameters. Because such experiments may be performed in any of a variety of types of calorimeters with varying degrees of calorimetric accuracy, it is important that the reporting of such results include an assessment of accuracy and precision. The term stands in contrast to the main emphasis in enthalpimetric analysis.

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2490

calorimetry

A general term describing any experiment in which heat is measured as some chemical reaction or physical process occurs.

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2488

candela

SI base unit for luminous intensity (symbol: cd). The candela is the luminous intensity, in a given direction, of a source that emits monochromatic radiation of frequency 540×10^{12} hertz and that has a radiant intensity in that direction of $(\frac{1}{683})$ watt per steradian.

Source:
Green Book, 2nd ed., p. 70
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 964

canonical rate constant

The rate constant for a system in which the reactants are in thermal equilibrium at a given temperature. In statistical mechanics the expression 'canonical ensemble' is used to refer to a closed system in thermal equilibrium, the species being present in a statistical distribution. By contrast, a microcanonical ensemble is composed of systems all having the same energy: a canonical ensemble therefore consists of a statistical distribution of microcanonical ensembles. The canonical or thermal rate constant can be obtained from the microcanonical rate constant by summing over the energy, taking into account the statistical distribution.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 155

canonical variational transition-state theory (CVTST)

A development of transition-state theory in which the position of the dividing surface is varied so as to minimize the rate constant at a given temperature.
See also: microcanonical variational transition-state theory

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 155

capacitance hygrometer

Hygrometer using the capacitance variations of a capacitor whose dielectric medium consists of the gas or of a material in contact with this gas.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

capacitance, *C*

of a plate capacitor

The charge on a plate divided by the potential difference between the plates.

Source:
Green Book, 2nd ed., p. 14
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 964

capillary column

in chromatography

A general term for columns having a small diameter. A capillary column may contain a packing or have the stationary phase supported on its inside wall. The former case corresponds to packed capillary column while the latter case corresponds to an open-tabular column. Due to the ambiguity of this term its use without an adjective is discouraged.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831

capillary condensation

Capillary condensation is said to occur when, in porous solids, multilayer adsorption from a vapour proceeds to the point at which pore spaces are filled with liquid separated from the gas phase by menisci. The concept loses its sense when the dimensions of the pores are so small that the term meniscus ceases to have a physical significance. Capillary condensation is often accompanied by hysteresis.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 588

See also:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

captodative effect

Effect on the stability of a carbon-centred radical determined by the combined action of a captor (electron withdrawing) and a dative (electron releasing) substituent, both attached to the radical centre. The term is also used for certain unsaturated compounds.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1092

capture

A process in which an atomic or nuclear system acquires an additional particle. In general, a specification is added of the type of the captured particle or its energy.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

capture cross-section

The cross-section for capture.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

capture γ-radiation

The γ-radiation emitted in radiative capture.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

carbaboranes

A class of boron compound of general formula $[(CH)_a(BH)_mH_b]^c$ where c can be positive, negative or zero. The CH groups occupy polyhedron vertices, and other hydrogen atoms are either bridging or terminal.
Note:
The contraction 'carboranes' is also well established as the generic name for this class of compound.

Source:
Red Book, p. 228
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1326

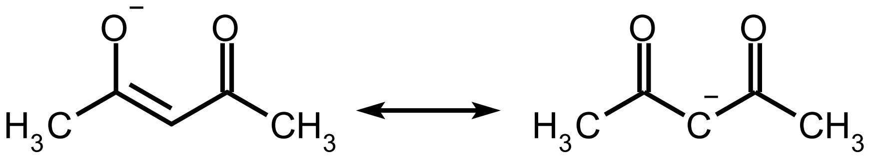
carbamates

Salts or esters of carbamic acid, $H_2NC(=O)OH$, or of *N*-substituted carbamic acids $R_2NC(=O)OR'$, (R' = hydrocarbyl or a cation). The esters are often called urethanes or urethans, a usage that is strictly correct only for the ethyl esters.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1323

carbanion

Generic name for anions containing an even number of electrons and having an unshared pair of electrons on a tervalent carbon atom (e.g. Cl_3C^- or $HC{\equiv}C^-$) or — if the ion is mesomeric (see mesomerism) — having at least one significant contributing structure with an unshared pair of electrons on a tervalent carbon atom, for example:



See also: radical ion

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1092

See also:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1324

carbena [obsolete]

This prefix is now rejected. It has been used in the past, especially in cyclic systems, to name carbenes, e.g. 'carbenacycloheptane', now cycloheptylidene.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1324

carbene analogues

The electrically neutral mononuclear hydrides of group 14 having two non-bonding electrons, the electrically neutral mononuclear hydrides of group 15 having four non-bonding electrons, and also the compound HB:. The names of a number of these are shown below.

RB:	boranylidenes	RAs:	arsanylidenes
RN:	nitrenes	R_2Sn:	stannylidenes
R_2Si:	silylenes	RSb:	stibanylidenes
RP:	phosphanylidenes	R_2Pb:	plumbylidenes
R_2Ge:	germylidenes		

Note that if R = H, these compounds are parent hydrides; derivatives formed by substitution are named accordingly. However, if the substituent's first atom, bearing the free valence, is of the same element as the atom of the carbene analogue, other parent compounds may be required (see carbenes), e.g. HN: nitrene; CH_3N: methylnitrene; H_2NN: diazanylidene (synonym isodiazene, not aminonitrene).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1324

carbene radical anions

Species $R_2C^{\cdot\cdot\cdot -}$, having three non-bonding electrons, formally derived by addition of an electron to a carbene.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1324

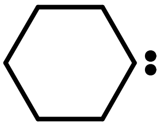
carbene radical cations

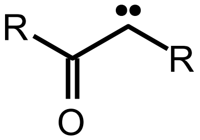
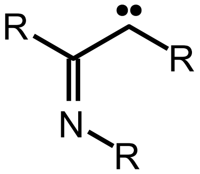
Species $R_2C^{\cdot +}$ having one non-bonding electron, formally derived by subtraction of an electron from a carbene, e.g. $H_2C^{\cdot +}$ methyliumyl.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1324

carbenes

The electrically neutral species H_2C: and its derivatives, in which the carbon is covalently bonded to two univalent groups of any kind or a divalent group and bears two nonbonding electrons, which may be spin-paired (singlet state) or spin-non-paired (triplet state). In systematic name formation, carbene is the name of the parent hydride $:CH_2$ hence, the name dichlorocarbene for $:CCl_2$. However, names for acyclic and cyclic hydrocarbons containing one or more divalent carbon atoms are derived from the name of the corresponding all-λ^4-hydrocarbon using the suffix -ylidene. E.g. prop-2-en-1-ylidene, $H_2C{=}CHCH$: ethenylidene, $H_2C{=}C$:; cyclohexylidene,



Subclasses of carbenes include acyl carbenes  , imidoyl carbenes,  and vinyl carbenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1324

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1092

carbenium centre

The three-coordinate carbon atom in a carbenium ion to which the excess positive charge of the ion (other than that located on heteroatoms) may be formally considered to be largely attributed, i.e. which has one vacant p-orbital. (N.B. It is not always possible to uniquely identify such an atom.) This formal attribution of charge often does not express the real charge distribution.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1092

carbenium ion

A generic name for carbocations, real or hypothetical, that have at least one important contributing structure containing a tervalent carbon atom with a vacant p-orbital. (The name implies a protonated carbene or a substitution derivative thereof.) The term was proposed (and rejected) as a replacement for the traditional usage of the name carbonium ion. To avoid ambiguity, the name should not be used as the root for the systematic nomenclature of carbocations. The corresponding difficulty confused carbonium ion nomenclature for many years. For example, the term 'ethylcarbonium ion' has at times been used to refer either to $CH_3CH_2^+$ (ethyl cation) or (correctly) to $CH_3CH_2CH_2^+$ (propyl cation).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1092
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1324
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1092

carbenoids

Complexed carbene-like entities that display the reactivity characteristics of carbenes, either directly or by acting as sources of carbenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1092

carbinolamines **[obsolete]**

An obsolete term for hemiaminals.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbinols **[obsolete]**

An obsolete term for substituted methanols, in which the name carbinol is synonymous with methanol.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbinyl cations **[obsolete]**

An obsolete term, derived from carbinol, once used for carbenium ions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbo-reduction

Process in which a metal oxide is reduced in the presence of carbon or a carbon-containing compound.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1821

carbocation

A cation containing an even number of electrons with a significant portion of the excess positive charge located on one or more carbon atoms. This is a general term embracing carbenium ions, all types of carbonium ions vinyl cations, etc. Carbocations may be named by adding the word 'cation' to the name of the corresponding radical. Such names do not imply structure (e.g. whether three-coordinated or five-coordinated carbon atoms are present).
See also: bridged carbocation, radical ion

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1093
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbocyclic compounds

Cyclic compounds in which all of the ring members are carbon atoms, e.g. 1,2-dihydronaphthalene.
See also: homocyclic compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbodiimides

Carbodiimide, HN=C=NH, and its hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbohydrates

Originally, compounds such as aldoses and ketoses having the stoichiometric formula $C_n(H_2O)_n$, hence 'hydrates of carbon'. The generic term carbohydrate includes monosaccharides, oligosaccharides and polysaccharides as well as substances derived from monosaccharides by reduction of the carbonyl group (alditols), by oxidation of one or more terminal groups to carboxylic acids, or by replacement of one or more hydroxy group(s) by a hydrogen atom, an amino group, thiol group or similar groups. It also includes derivatives of these compounds.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbon

Element number 6 of the periodic table of elements (electronic ground state $1s^2\ 2s^2\ 2p^2$). For a description of the various types of carbon as a solid the term carbon should be used only in combination with an additional noun or a clarifying adjective.
See also: amorphous carbon, carbon fibres, carbon material, glass-like carbon, graphitic carbon, non-graphitic carbon, pyrolytic carbon

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 479

carbon artifact

An 'artificially produced' solid body which consists mainly of carbonaceous material in a distinct shape.
Note:
Sometimes this term is also used for artificially (in the sense of technically) produced non-shaped carbon materials such as coke, blacks, etc. This application of the term carbon artifact is not recommended. Synonyms to the term carbon artifact are: 'artificial carbon article' or 'artificial carbon body'.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 479

carbon black

An industrially manufactured colloidal carbon material in the form of spheres and of their fused aggregates with sizes below $1000\ \mathrm{nm}$.
Note:
Carbon black is a commercial product manufactured by thermal decomposition, including detonation, or by incomplete combustion of carbon hydrogen compounds and has a well-defined morphology with a minimum content of tars or other extraneous materials. For historical reasons, however, carbon black is popularly but incorrectly regarded as a form of soot. In fact, in many languages, the same word is used to designate both materials. Carbon black is manufactured under controlled conditions, whereas soot is randomly formed. They can be distinguished on the basis of tar, ash content and impurities. Attempts in the literature to create a general term, 'aciniform carbon', which would cover both carbon black and soot, are not yet generally accepted.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 479
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2178

carbon cenospheres

Porous or hollow carbonaceous sphere-like particles (frequently in the size range of a few to several hundreds of μ m diameter) formed during pyrolysis, also in the course of combustion, of carbonaceous liquid droplets (e.g. heavy fuel) or solid particles (e.g. coal).

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 480

carbon cloth

A textile material consisting of carbon fibres oriented at least in two directions. Carbon cloth is not necessarily woven.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 480

carbon dioxide laser (CO_2 laser)

A continuous or pulsed source of coherent radiation normally tunable through the CO_2 vibration–rotation band centred near $10.6\ \mu m$.
See also: gas lasers, laser

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2233

carbon electrode

Also contains definition of: graphite electrode

An electrode for an electrical application. In its green state it comprises granular carbon material bound with pitch. The granular carbon material may be either needle coke, fine-grained or isotropic coke or reclaimed graphite powder. Electrodes for use in steel production can only be manufactured from needle coke, and the green electrodes are fired at temperatures above around $2800\ K$ to produce highly graphite electrodes. The other granular carbon materials may be used for aluminium electrodes where the duty is not so severe, and the green electrodes are generally fired to lower temperatures.
Note:

In both cases it is essential that the granular carbons and the pitch binders used in the production of the green electrodes have a low sulfur content as the release of sulfur during the high-temperature firing can lead to the production of significant porosity.
See also: puffing, graphitic carbon, graphitization heat treatment, isotropic carbon

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 480

carbon felt

A textile material consisting of, in approximation, randomly oriented and intertwined carbon fibres.
Note:
Carbon felts are usually fabricated by carbonization of organic felts but they can also be produced from short carbon fibres.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 481

carbon fibre

Fibres (filaments, tows, yarns, rovings) consisting of at least 92% (mass fraction) carbon, usually in the non-graphitic state.
Note:
Carbon fibres are fabricated by pyrolysis of organic precursor fibres or by growth from gaseous hydrocarbons. The use of the term graphite fibres instead of carbon fibres as often observed in the literature is incorrect and should be avoided. The term graphite fibres is justified only if three-dimensional crystalline order is confirmed, e.g. by X-ray diffraction measurements.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 480

carbon fibre fabrics

Woven textile materials made of carbon fibres.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 481

carbon fibres type HM

Carbon fibres type HM (high modulus) are carbon fibres with a value of Young's modulus (tensile modulus) larger than $300\ \mathrm{GPa}$ (nearly 30% of the C_{11} elastic constant of a graphite single crystal).
Note:

The level of the tensile modulus of carbon fibres is controlled by the degree of preferred orientation of the layer planes in the direction parallel to the fibre axis. C_{11}, the elastic constant of graphite single crystals in the direction of the layer planes, is 1060 ± 20 GPa. In general, the ratio of tensile strength to tensile modulus is smaller than 1×10^{-2} for carbon fibres type HM (but the tensile strength is influenced by flaws in the fibres and may be improved in the future). Carbon fibres type UHM (ultra-high modulus) have moduli of elasticity in excess of 600 GPa, surpassing 50% of the theoretical C_{11} number. Such high values of Young's modulus can be achieved most readily in mesophase pitch-based carbon fibres (MPP-based carbon fibres).

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 481

carbon fibres type HT

Carbon fibres type HT are carbon fibres with values of Young's modulus between 150 and 275 to 300 GPa. The term HT, referring to high tensile strength, was early applied because fibres of this type display the highest tensile strengths.
Note:
The disposition of boundaries between the fibre types is somewhat arbitrary. For carbon fibres type HT, the values of the strength-to-stiffness ratio are typically larger than 1.5×10^{-2}. The tensile strength of carbon fibres is flaw-controlled, however, and therefore the measured values increase strongly as the diameter of the filaments is decreased.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 481

carbon fibres type IM

Carbon fibres type IM (intermediate modulus) are related to carbon fibres type HT because of the comparable values of tensile strength, but are characterized by greater stiffness (Young's modulus up to approximately 35% of the theoretical C_{11} value).

Note:
The tensile modulus (Young's modulus) varies between *ca.* 275 and 350 GPa, but the disposition of the boundaries is somewhat arbitrary. The relatively high ratio of tensile strength to tensile modulus, typically above 1×10^{-2}, in carbon fibres type IM, in spite of an increase of Young's modulus, requires a further increase of strength, which is achievable by a significant reduction of the monofilament diameter down to about 5 μm. Such small filament diameters are typical of carbon fibres type IM.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 482

carbon fibres type LM

Carbon fibres type LM (low modulus) are carbon fibres with isotropic structure, tensile modulus values as low as 10% of the C_{11} values of the graphite single crystal, and low strength values.

Note:

The term carbon fibres type LM is sometimes used for various types of isotropic carbon fibres known as pitch-based or rayon-based carbon fibres that have not been subjected to hot-stretching. Such fibres are not used for reinforcement purposes in high-performance composites.

Source:

PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 482

carbon fibres type UHM

Carbon fibres type UHM (ultra-high modulus) designates a class of carbon fibres having very high values of Young's modulus larger than $600\ \mathrm{GPa}$ (i.e. greater than 55% of the theoretical C_{11} value of graphite).

Source:

PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 482

carbon loading

of the packing material

in liquid chromatography

Mass fraction of the packing material which is carbon. Usually taken as a guide to the extent of alkyl substitution on the surface. Usually reported as percentage carbon determined using elemental analysis.

Source:

PAC, 1997, *69*, 1475 *(Classification and characterization of stationary phases for liquid chromatography: Part I. Descriptive terminology (IUPAC Recommendations 1997))* on page 1477

carbon material

A solid high in content of the element carbon and structurally in a non-graphitic state.

Note:

The use of the term carbon as a short term for a material consisting of non-graphitic carbon is incorrect. The use of the term carbon without a second noun or a clarifying adjective should be restricted to the chemical element carbon. The term carbon can be used in combination with other nouns or clarifying adjectives for special types of carbon materials (carbon electrode, carbon fibres, pyrolytic carbon, glass-like carbon and others).

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 482

carbon mix

A mixture of filler coke, e.g. grains and/or powders of solid carbon materials and a carbonaceous binder and selected additives, prepared in heated mixers at temperatures in the range of $410-445\ \mathrm{K}$ as a preliminary step for the formation of shaped green bodies.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 483

carbonaceous mesophase

A liquid-crystalline state of pitch which shows the optical birefringence of disc-like (discotic) nematic liquid crystals. It can be formed as an intermediate phase during thermolysis (pyrolysis) of an isotropic molten pitch or by precipitation from pitch fractions prepared by selective extraction. Generally, the spherical mesophase precipitated from a pyrolysing pitch has the Brooks and Taylor structure. With continuous heat treatment the carbonaceous mesophase coalesces to a state of bulk mesophase before solidification to green coke with further loss of hydrogen or low-molecular-weight compounds.
Note:
In the formation of carbonaceous mesophase by thermolysis (pyrolysis) of isotropic molten pitch, the development of a liquid-crystalline phase is accompanied by simultaneous aromatic polymerization reactions. The reactivity of pitch with increasing heat treatment temperature and its thermosetting nature are responsible for the lack of a true reversible thermotropic phase transition for the bulk mesophase in most pitches. Due to its glass-like nature most of the liquid-crystalline characteristics are retained in the super-cooled solid state.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 483

carbonitriles

In systematic nomenclature, the suffix -carbonitrile is used to name compounds $RC{\equiv}N$ where the suffix includes the carbon atom of the –CN. However, carbonitrile is not a class name for nitriles.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbonium ion

The term should be used with great care since several incompatible meanings are currently in use. It is not acceptable as the root for systematic nomenclature for carbocations.

1. In most of the existing literature the term is used in its traditional sense for what is here defined as carbenium ion.
2. A carbocation, real or hypothetical, that contains at least one five-coordinate carbon atom.
3. A carbocation, real or hypothetical, whose structure cannot adequately be described by two-electron two-centre bonds only. (The structure may involve carbon atoms with a coordination number greater than five.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1093
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbonization

A process by which solid residues with increasing content of the element carbon are formed from organic material usually by pyrolysis in an inert atmosphere.
Note:
As with all pyrolytic reactions, carbonization is a complex process in which many reactions take place concurrently such as dehydrogenation, condensation, hydrogen transfer and isomerization. It differs from coalification in that its reaction rate is faster by many orders of magnitude. The final pyrolysis temperature applied controls the degree of carbonization and the residual content of foreign elements, e.g. at $T \sim 1200\ \mathrm{K}$ the carbon content of the residue exceeds a mass fraction of 90 wt.%, whereas at $T \sim 1600\ \mathrm{K}$ more than 99 wt.% carbon is found.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 484

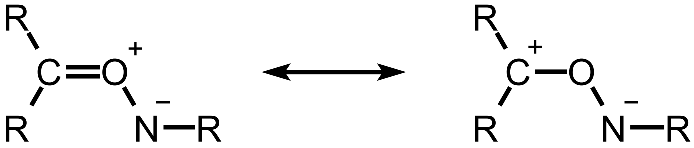
carbonyl compounds

1. Compounds containing the carbonyl group, C=O. The term is commonly used in the restricted sense of aldehydes and ketones, although it actually includes carboxylic acids and derivatives.
   See also: oxo compounds
2. Metal carbonyls, in which carbon monoxide is a formal ligand.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbonyl imides

1,3-Dipolar compounds having the structure:



See also: oxonium ylides (2)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbonyl imines [obsolete]

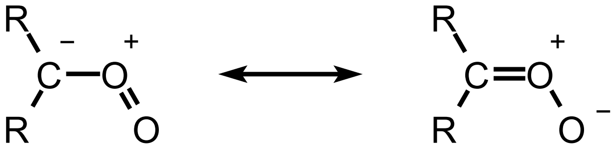
An undesirable synonym for carbonyl imides.
See: ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbonyl oxides

Synonym: peroxo compounds

1,3 Dipolar compounds having the structure

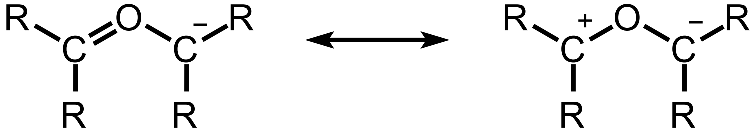


. Also called peroxo compounds.
See also: oxonium ylides (2)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbonyl ylides

1,3-Dipolar compounds having the structure



.

See also: oxonium ylides (2)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1325

carbon–carbon composite

A carbon fibre-reinforced carbon matrix material. The carbon matrix phase is typically formed by solid, liquid or gaseous pyrolysis of an organic precursor material. The matrix is either a graphitizable carbon or non-graphitizable carbon, and the carbonaceous reinforcement is fibrous in form. The composite may also contain other components in particulate or fibrous forms.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 480

carboranes

See: carbaboranes

Source:
Red Book, p. 228
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1326

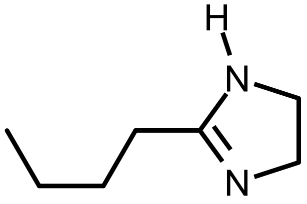
carboxamides

Amides of carboxylic acids, having the structure $RC(=O)NR_2$. The term is used as a suffix in systematic name formation to denote the $–C(=O)NH_2$ group including its carbon atom.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1326

carboxamidines

Compounds having the structure $RC(=NR)NR_2$. The term is used as a suffix in systematic nomenclature to denote the $–C(=NH)NH_2$ group including its carbon atom, e.g. acetamidine, $CH_3C(=NH)NH_2$; 2-butyl-4,5-dihydroimidazole:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1326

carboxylic acids

Oxoacids having the structure RC(=O)OH. The term is used as a suffix in systematic name formation to denote the –C(=O)OH group including its carbon atom.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1326

carbylamines [obsolete]

An obsolete term, which should not be used, for isocyanides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1326

carbynes

The neutral species $HC^{\cdot\cdot\cdot}$ and its derivatives formed by substitution in which a univalent carbon atom is covalently bonded to one group and also bears three nonbonding electrons. (This term carries no implication about spin-pairing).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1326

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1093

carbynium ions

The cationic species $H_2C^{\cdot +}$ or substitution derivatives thereof, formally derived by adding a hydron to a carbyne or subtracting an electron from a carbene.

Source:
PAC, 1996, *68*, 1321 *(A new approach to enhancing the efficiency and specificity of interaction in duplexes by the use of tandem structure)* on page 1326

carotenes

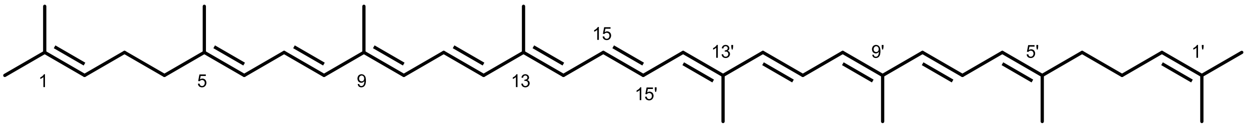
Hydrocarbon carotenoids (a subclass of tetraterpenes).

See also: terpenes

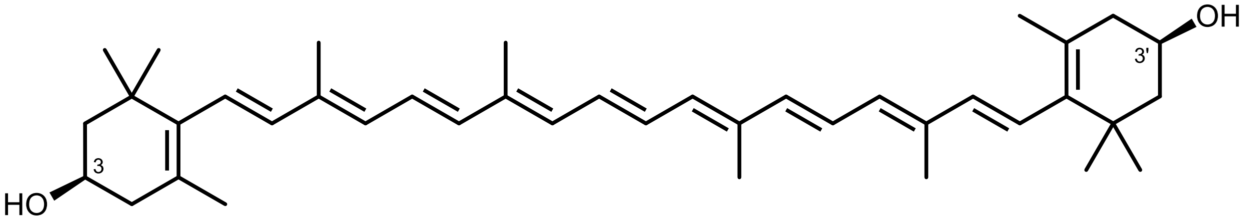
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1326

carotenoids

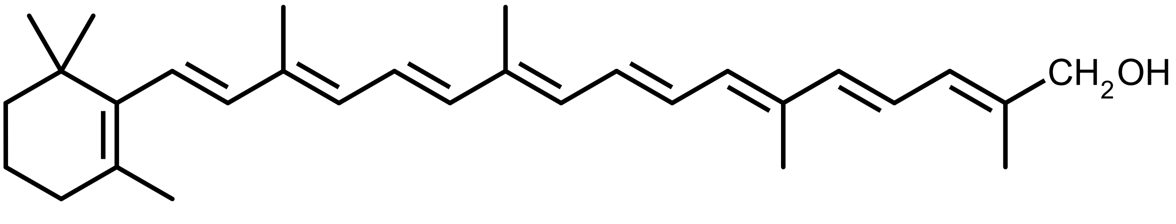
Tetraterpenoids (C_{40}), formally derived from the acyclic parent, Ψ,Ψ-carotene I by hydrogenation, dehydrogenation, cyclization, oxidation, or combination of these processes. This class includes carotenes, xanthophylls and certain compounds that arise from rearrangement of the skeleton of I or by loss of part of this structure. Retinoids are excluded.



lycopene, ψ,ψ-carotene (I)



zeaxanthin, β,β-carotene-3,3'-diol (a xanthophyll)



8'-apo-β-caroten-8'-ol

See also: retro

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1326

carrier

A substance in appreciable amount which, when associated with a trace of a specified substance, will carry the trace with it through a chemical or physical process.

See also: support *of a catalyst*

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

See also:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

carrier atom

in organic reaction mechanisms

A participant atom which is neither core nor peripheral and which carries other groups to and from the molecule containing the core atom(s) but which does not itself become covalently attached to that molecule.

Source:
PAC, 1989, *61*, 23 *(System for symbolic representation of reaction mechanisms (Recommendations 1988))* on page 27

carrier gas

A gas introduced in order to transport a sample for analytical purposes. In gas chromatography it is the gas which is passed continuously through the column and whose passage promotes the elution of the components of the sample. The carrier gas together with the portions of the sample present in this phase constitutes the mobile phase.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2178
Orange Book, p. 97
Orange Book, p. 136

carrier

in radioanalytical chemistry

A substance in appreciable amount which, when associated with a tracer of a specified substance, will carry the tracer with it through a chemical or physical process, or prevent the tracer from undergoing nonspecific processes due to its low concentration.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

carrier protein

1. Protein to which a specific ligand or hapten is conjugated.
2. Unlabeled protein introduced into an assay at relatively high concentrations which distributes in a fractionation process in the same manner as labeled protein analyte, present in very low concentrations.
3. Protein added to prevent non-specific interaction of reagents with surfaces, sample components, and each other.
4. Protein found in cell membranes, which facilitates transport of a ligand across the membrane.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1043

carrier-free [obsolete]

See: no carrier added, which term should be preferred

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

carry-over

Also contains definition of: carry-over effect

A process by which materials are carried into a reaction mixture to which they do not belong. These materials can be either parts of a specimen, or reagents including the diluent or wash solution. In such cases, carry-over means the transfer of material (specimen or reagents) from one container, or from one reaction mixture, to another one. It can be either unidirectional or bidirectional in a series of specimens or assays. The term carry-over effect is used for carry-over from specimen to specimen.

Source:
PAC, 1991, *63*, 301 *(Proposals for the description and measurement of carry-over effects in clinical chemistry (Recommendations 1991))* on page 302
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663

cascade impactor

An instrument used for the classification of aerosols according to size and for possible subsequent chemical analysis. Air is drawn through a series of orifices of decreasing size; the air flow is normal to collecting surfaces on which aerosols are collected by inertial impaction. The particles, separated stepwise by their momentum differences into a number of size ranges, are collected simultaneously.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

catabolism

1. Reactions involving the oxidation of organic substrates to provide chemically available energy (e.g. ATP) and to generate metabolic intermediates.
2. Generally, the process of breakdown of complex molecules into simpler ones, often providing biologically available energy.

See also: anabolism

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2013
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 149

catabolite repression

A decrease in the activity of certain auxiliary catabolic enzymes when a surplus of an (easily metabolizable) substrate is available. Commonly this effect is caused by glucose (glucose repression) or by metabolites produced from glucose.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 149

catalase

A hemeprotein which catalyses the disproportionation of dihydrogen peroxide to O_2, and water; it also catalyses the oxidation of other compounds , such as ethanol, by dihydrogen peroxide. Note. A non-hemeprotein containing a dinuclear managanese cluster with catalase activity is often called pseudocatalase.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1262

catalymetric titration

A titration process, which involves a catalyst, where the end-point is detected by the sudden increase or decrease of the rate of a reaction.

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2293

catalysed rate of reaction, ξ_{cat}

The observed rate of reaction, ξ, minus the spontaneous rate of reaction, ξ_0, observed under otherwise similar conditions in the absence of added catalytic material.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2464

catalysis

The action of a catalyst.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1093

catalyst

Also contains definitions of: heterogeneous catalysis, homogeneous catalysis

A substance that increases the rate of a reaction without modifying the overall standard Gibbs energy change in the reaction; the process is called catalysis. The catalyst is both a reactant and product of the reaction. The words catalyst and catalysis should not be used when the added substance reduces the rate of reaction (see inhibitor). Catalysis can be classified as homogeneous catalysis, in which only one phase is involved, and heterogeneous catalysis, in which the reaction occurs at or near an interface between phases. Catalysis brought about by one of the products of a reaction is called autocatalysis. Catalysis brought about by a group on a reactant molecule itself is called intramolecular catalysis. The term catalysis is also often used when the substance is consumed in the reaction (for example: base-catalysed hydrolysis of esters). Strictly, such a substance should be called an activator.
See also: autocatalytic reaction, bifunctional catalysis, catalytic coefficient, electron-transfer catalysis, general acid catalysis, general base catalysis, intramolecular catalysis, micellar catalysis, Michaelis-Menten kinetics, phase-transfer catalysis, pseudo-catalysis, rate of reaction, specific catalysis

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 155

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1093
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2293
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2178

catalyst ageing

Catalyst deactivation resulting from changes in the structure or in the texture of the catalyst. Changes of this kind are usually irreversible and the catalyst cannot be regenerated.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 84

catalyst decay

Synonym: catalyst deactivation

The conversion in a catalytic reaction performed under constant conditions of reaction often decreases with time of run or time on stream. This phenomenon is called catalyst deactivation or catalyst decay.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 83

catalyst

in solvent extraction

A substance included in the solvent to increase the rate of transfer without affecting the position of equilibrium. The term accelerator may also be used but kinetic synergist is not recommended.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2380

catalytic activity concentration, b

Also contains definition of: catalytic concentration

Catalytic activity of the component divided by the volume of the system.
Notes:
1. In clinical chemistry litre is recommended as unit for the volume.
2. In clinical chemistry the component is usually an enzyme.
3. The term catalytic concentration is accepted for use in clinical chemistry.
4. Use of the term level as a synonym for concentration is deprecated.
5. In describing a quantity, concentration must be clearly differentiated from content.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 964

catalytic activity content, z/m

Also contains definition of: catalytic content

Catalytic activity of the component divided by the mass of the system.
Notes:

1. In clinical chemistry the component is usually an enzyme.
2. The term catalytic content is accepted for use in clinical chemistry.
3. Use of the term level as a synonym for concentration is deprecated.
4. In describing a quantity, content must be clearly differentiated from concentration.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 964

catalytic activity fraction
Also contains definition of: catalytic fraction

of an isozyme

Quotient of the catalytic activity of the isozyme and the catalytic activity of all the isozymes of the same enzyme in the system.
Notes:
1. The term catalytic fraction is accepted for use in clinical chemistry.
2. The definition is based on the definitions of catalytic activity and fraction.
3. The definition also applies to other multiple forms of an enzyme that are not isoenzymes.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 964

catalytic activity, z
of an enzyme

Increase in the rate of reaction of a specified chemical reaction that an enzyme produces in a specific assay system.
See: rate of reaction

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 964
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

catalytic coefficient

If the rate of reaction, v, is expressible in the form:

$$v = \left(k_0 + \sum_i k_i \, [C_i]^{n_i}\right) [\mathrm{A}]^{\alpha} \, [\mathrm{B}]^{\beta} \ldots$$

where A, B, ... are reactants and C_i represents one of a set of catalysts, then the proportionality factor k_i is the catalytic coefficient of the particular catalyst C_i. Normally the partial order of reaction n_i with respect to a catalyst is unity, so that k_i is an (α + β + ... + 1)th order rate coefficient. The proportionality factor k_0 is the ($\alpha + \beta + ...$)th order rate coefficient of the uncatalysed component of the total reaction. For example, if there is catalysis by hydrogen and hydroxide ions, and the rate constant can be expressed in the form:

$$k = k_0 + k_{H^+}[H^+] + k_{OH^-}[OH^-],$$

then k_{H^+} and k_{OH^-} are the catalytic coefficients for H^+ and OH^-, respectively. The constant k_0 relates to the uncatalysed reaction.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 156
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1093

catalytic cracking

See: cracking

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

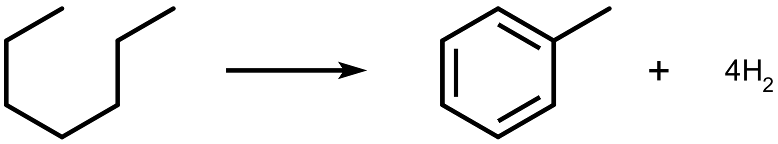
catalytic current

The faradaic current that is obtained with a solution containing two substances **B** and **A** may exceed the sum of the faradaic currents that would be obtained with **B** and **A** separately, but at the same concentrations and under the same experimental conditions. In either of the two following situations the increase is termed a catalytic current. **B** is reduced or oxidized at the electrode-solution interface to give a product **B'** that then reduces or oxidizes **A** chemically. The reaction of **B** with **A** may yield either **B** or an intermediate in the overall half-reaction by which **B'** was obtained from **B**. In this situation the increase of current that results from the addition of **A** to a solution of **B** may be termed a regeneration current. The presence at the electrode-solution interface of one substance, which may be either **A** or the product **A'** of its reduction or oxidation, decreases the over-potential for the reduction or oxidation of **B**. In either case the magnitude of the catalytic current depends on the applied potential. If the current observed with a mixture of **A** and **B** is smaller than the sum of the separate currents, the term non-additive current should be used.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1494

catalytic dehydrocyclization

A reaction in which an alkane is converted into an aromatic hydrocarbon and hydrogen. For example,



Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 86

catalytic domain

of a polypeptide

Any part of a polypeptide chain that possesses a catalytic function. It may contain more than one structural domain.

Source:
White Book, p. 107

catalytic graphitization

The transformation of non-graphitic carbon into graphite by heat treatment in the presence of certain metals or minerals.
Note:
Catalytic graphitization gives a fixed degree of graphitization at lower temperature and/or for a shorter heat treatment time than in the absence of the catalytic additives (or a higher degree of graphitization at fixed heat treatment conditions). Often it involves dissolution of carbon and precipitation of graphite at the catalyst particles so that non-graphitizing carbons can be graphitized by this procedure.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 484

catalytic hydrocracking

A process similar to catalytic cracking in its industrial purpose but effected under hydrogen pressure and on a catalyst containing an ingredient with a hydrogenating function.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 86

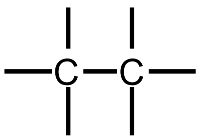
catalytic hydrodesulfurization

A process in which, in the presence of hydrogen, sulfur is removed as hydrogen sulfide.

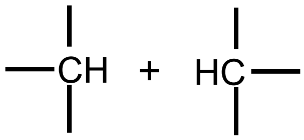
Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 86

catalytic hydrogenolysis

Ordinarily, a reaction in which A + H_2 gives B.

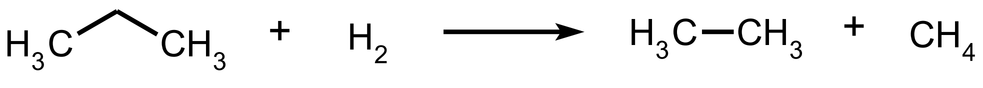


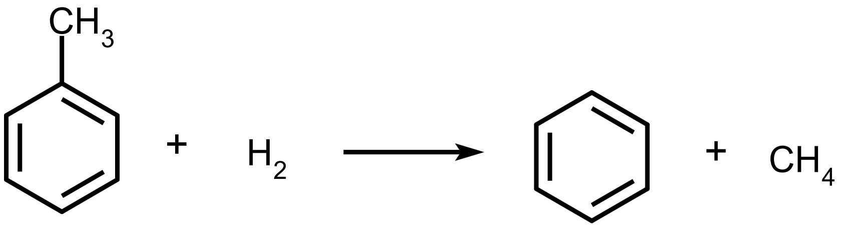
A

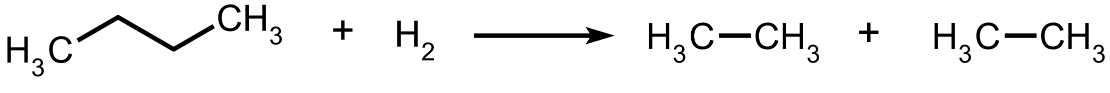


B

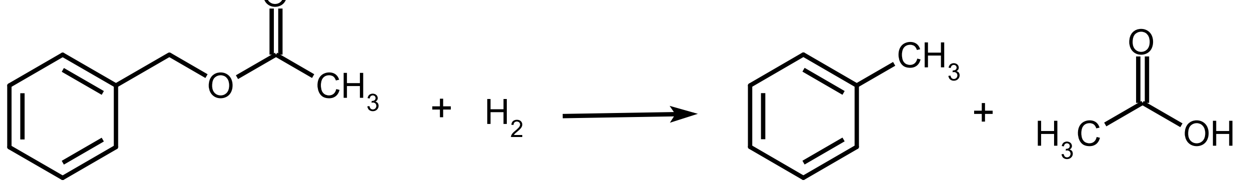
For example,

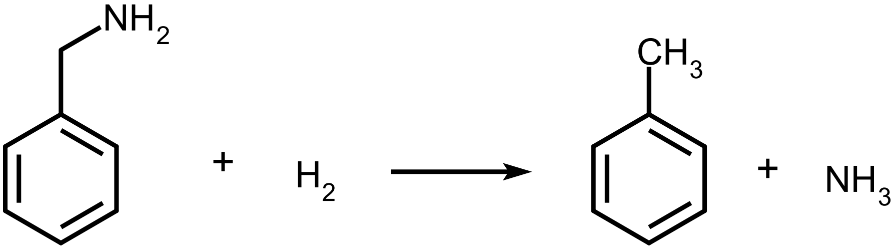






The term may also be used for cleavage of bonds other than A, e.g.





Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 86

catalytic methanation

A process for removing carbon monoxide from gas streams or for producing methane by the reaction

$$CO + 3H_2 \longrightarrow CH_4 + H_2O$$

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 86

catalytic reforming

A process for increasing the octane number of naphthas. It involves isomerization of alkanes, dehydrogenation of cyclohexanes to aromatic hydrocarbons, isomerization and dehydrogenation of alkylcyclopentanes, and dehydrocyclization of alkanes.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 86

catalytic thermometric titration [obsolete]

See: thermometric titration

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2490

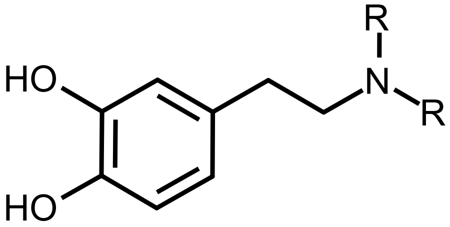
cataphoresis [obsolete]

See: electrophoresis

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 619

catecholamines

4-(2-Aminoethyl)pyrocatechol [4-(2-aminoethyl)benzene-1,2-diol] and derivatives formed by substitution.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1327

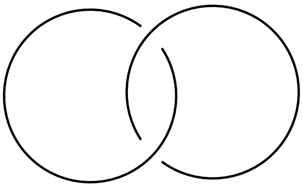
catena-

An affix used in inorganic nomenclature to denote a chain structure; often used to designate linear polymeric substances.

Source:
Red Book, p. 245
Blue Book, p. 464

catenanes (catena compounds)

Hydrocarbons having two or more rings connected in the manner of links of a chain, without a covalent bond. More generally, the class catena compounds embraces functional derivatives and hetero analogues, e.g:



a [2]catenane

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1327

cathode

Electrode at which reduction takes place.

Source:
Green Book, 2nd ed., p. 59

cathodic transfer coefficient, α_c

For a reaction with a single rate-determining step

$$\frac{\alpha_c}{\nu} = -\frac{R\,T}{n\,F}\left(\frac{\partial(\ln(\,|\,I_c\,|\,))}{\partial E}\right)_{T,p,c_i,...}$$

where α_c is the cathodic transfer coefficient (number), R is the gas constant, T is the thermodynamic temperature, and ν the stoichiometric number giving the number of identical activated complexes formed and destroyed in the completion of the overall reaction as formulated with the transfer of n electrons.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 515

cation

A monoatomic or polyatomic species having one or more elementary charges of the proton.

Source:
Red Book, p. 102

cation exchange

The process of exchanging cations between a solution and a cation exchanger.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 854

cation exchanger

Ion exchanger with cations as counter-ions. The term cation-exchange resin may be used in the case of solid organic polymers. The acid form of a cation exchanger is the ionic form of a cation exchanger in which counter-ions are hydrogen ions (H-form) or the ionogenic groups have added a proton forming an undissociated acid.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 855

cation-exchange polymer

See also: ion-exchange polymer

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2069

cationic polymer

Polymer composed of positively charged macromolecules and an equivalent amount of counter-anions.
Notes:
1. If a substantial fraction of constitutional units carries positive charges, then a cationic polymer is a polyelectrolyte.
2. The positive charges may be fixed on groups located in main chains as in an ionene or in pendant groups.
3. The term cationic polymer should not be used to denote a polymer prepared by cationic polymerization.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2069

cationic polymerization

An ionic polymerization in which the kinetic-chain carriers are cations.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2308

cationotropic rearrangement

See: tautomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1093

cationotropy

See: tautomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1093

cavitands

Compounds constrained by structure to having or accommodating a cavity large enough to host other molecules.
See: inclusion compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1327

cavity dumping

in photochemistry

Periodic removal of coherent radiation from a laser cavity.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2231

ceiling value (CV)

Airborne concentration of a potentially toxic substance which should never be exceeded in a worker's breathing zone.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1043

ceilometer

in atmospheric chemistry

An automatic, recording instrument for reading the height of the cloud-base.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2178

cell constant

of a conductivity cell

Defined as:

$$\kappa_{\text{cell}} = \kappa R$$

where R is the measured resistance of the cell and κ is the conductivity (formerly called the specific conductance).

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 511

cell error

in spectrochemical analysis

The error which results if the incident beam does not fall perpendicularly to the windows of the cell, or if the cell windows are contaminated or have some other imperfection.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1457

cell line

Defined unique population of cells obtained by culture from a primary source through numerous generations.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1043

Celsius temperature, t, θ

Thermodynamic temperature minus $273.15\ \mathrm{K}$, invariably expressed in the SI unit degree Celsius ($^\circ\mathrm{C}$) which is equal to the kelvin. Sometimes the misnomer centigrade temperature is used for Celsius temperature.

Source:
Green Book, 2nd ed., p. 48
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 965

centi

SI prefix for 10^{-2} (symbol: c).

Source:
Green Book, 2nd ed., p. 74

central atom

The atom in a coordination entity which binds other atoms or groups of atoms (ligands) to itself, thereby occupying a central position in the coordination entity.

Source:
Red Book, p. 146

centre

of a Mossbauer spectrum

The centre of a Mössbauer spectrum is defined as the Doppler-velocity at which the resonance maximum is (or would be) observed when all magnetic dipole, electric quadrupole, etc. hyperfine interactions are (or would be) absent. The contribution of the second order Doppler shift (δ_{T}) should be indicated, if possible.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 215

centrifugal barrier

In a reaction without an electronic energy barrier, or its reverse, the rotational energy of the transition state gives rise to a reaction barrier, which is known as the centrifugal barrier.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 156

centrifugal (centripetal) acceleration, a_{rot}

The acceleration of a component as a result of a uniform rotational motion. Centrifugal acceleration is a vector quantity.

Source:
PAC, 1994, *66*, 897 *(Quantities and units for centrifugation in the clinical laboratory (IUPAC Recommendations 1994))* on page 900
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 965

centrifugal force, F_{rot}

Fictitious force acting on a body as a result of centripetal acceleration.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 965

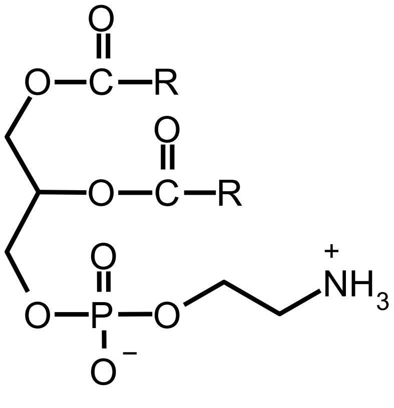
centrifugal radius, *r*

The radius at which a component is spinning at the end of the period of centrifugation. For a component sedimented from a dilute suspension, it can be equated with radius of rotation at the bottom of the centrifuge tube.

Source:
PAC, 1994, *66*, 897 *(Quantities and units for centrifugation in the clinical laboratory (IUPAC Recommendations 1994))* on page 901
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 965

cephalins (kephalins) [obsolete]

Compounds derived from glycerol in which a primary and the secondary hydroxy groups are esterified with long-chain fatty acids, and the remaining primary one with the mono(2-aminoethyl) ester of phosphoric acid, or with the monoserine ester of phosphoric acid. The term is not recommended. These compounds are preferably designated as (3-phosphatidyl)ethanolamines and (3-phosphatidyl)serines respectively.

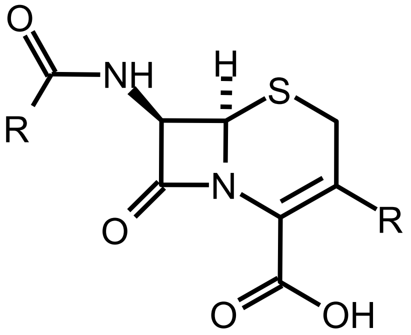


See also: phosphatidic acids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1327

cephalosporins

Cephems having the basic structure shown.

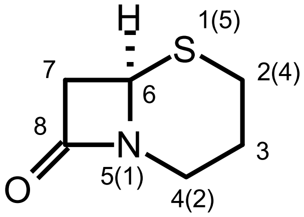


See also: cephams, cephems, penams, penems, penicillins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1327

cephams

Natural and synthetic antibiotics containing the 5-thia-1-azabicyclo[4.2.0]octan-8-one nucleus; generally assumed to have the 6*R* configuration, unless otherwise specified. The numbering used differs from that of the von Baeyer named bicyclic system. Where they differ, the von Baeyer numbering is shown in parentheses.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1327

cephems

2,3-Didehydrocephams: 5-thia-1-azabicyclo[4.2.0]oct-2-en-8-ones.
See: cephalosporins, cephams

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1327

ceramer

Chemically bonded hybrid material which is a crosslinked organic–inorganic polymer.
Note:
Ceramers are usually prepared by sol-gel processing of oligomers or polymers with reactive silyloxy substituents.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1810

ceramic

Rigid material that consists of an infinite three-dimensional network of sintered crystalline grains comprising metals bonded to carbon, nitrogen or oxygen.
Note:
The term ceramic generally applies to any class of inorganic, non-metallic product subjected to high temperature during manufacture or use.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1810

ceramic filter

A component of a stack sampling system which is suitable for high temperature use; also known as a ceramic thimble.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2178

ceramic precursor

Also contains definitions of: pre-ceramic, pre-ceramic material

Material that is converted to a ceramic through pyrolysis.
Note:
Examples include poly(dimethylsilanediyl), poly(carbasilane)s, poly(silazane)s, *etc.*

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1810

ceramic yield

Mass of ceramic expressed as a percentage of the mass of the ceramic precursor used in the ceramization process.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1810

ceramic-reinforced polymer

Polymer composite consisting of a polymer continuous phase and disperse phase domains of microscopic ceramic particles.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1810

ceramization

Process in which a ceramic precursor is converted into a ceramic.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1821

Cerenkov detector

A charged particle detector based on the Cerenkov effect.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

Cerenkov effect

Emission of radiation in the visible and ultraviolet spectrum arising when a charged particle crosses a medium with a velocity greater than that of light in the same medium.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

Cerenkov radiation

Radiation resulting from the Cerenkov effect.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

chain axis

of a polymer

The straight line parallel to the direction of chain extension, connecting the centres of mass of successive blocks of chain units, each of which is contained within an identity period.

Source:
Purple Book, p. 77

chain branching

When in a chain reaction there is a net increase in the number of chain carriers there is said to be chain branching. A simple example of a chain-propagating reaction leading to chain branching is:

$$\mathrm{O} + \mathrm{H_2} \longrightarrow \mathrm{OH} + \mathrm{H}$$

in which there is one chain carrier (an oxygen atom) on the left and two chain carriers (a hydrogen atom and a hydroxyl radical) on the right.
See also: degenerate chain branching

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 156

chain carrier

A species, such as an atom or free radical, which is involved in chain-propagating reactions is known as a chain carrier.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 156

(chain) conformational repeating unit

of a polymer

The smallest structural unit of a polymer chain with a given conformation that is repeated along that chain through symmetry operations.

Source:
Purple Book, p. 77

chain entanglement

Interlocking of polymer chains in a polymer material forming a transient or permanent network junction over the time-scale of the measurement.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1818

chain fission yield

The fraction of fissions giving rise to nuclei of a particular mass number.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

chain folding

in polymer crystals

The conformational feature in which a loop connects two parallel stems belonging to the same crystal.

Source:
Purple Book, p. 83

(chain) identity period

Synonyms: (chain) repeating distance, repeating distance

of a polymer

The shortest distance along the chain axis for translational repetition of the chain structure. The chain identity period is usually denoted by c. Synonymous with (chain) repeating distance.

Source:
Purple Book, p. 77

chain

in polymers

The whole or part of a macromolecule, an oligomer molecule or a block, comprising a linear or branched sequence of constitutional units between two boundary constitutional units, each of which may be either an end-group, a branch point or an otherwise-designated characteristic feature of the macromolecule.
Notes:

1. Except in linear single-strand macromolecules, the definition of a chain may be somewhat arbitrary.
2. A cyclic macromolecule has no end groups but may nevertheless be regarded as a chain.
3. Any number of branch points may be present between the boundary units.
4. Where appropriate, definitions relating to 'macromolecule' may also be applied to 'chain'.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2293

chain initiation

The process in a chain reaction that is responsible for the formation of a chain carrier.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 156

chain length, δ

In a chain reaction, the average number of times the closed cycle of reactions (involving the chain-propagating reactions) is repeated. It is equal to the rate of the overall reaction divided by the rate of the initiation reaction.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 157

chain polymerization

Also contains definition of: condensative chain polymerization

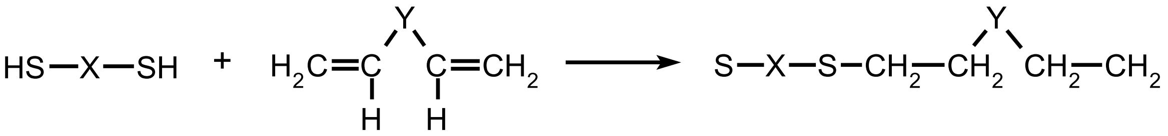
A chain reaction in which the growth of a polymer chain proceeds exclusively by reaction(s) between monomer(s) and reactive site(s) on the polymer chain with regeneration of the reactive site(s) at the end of each growth step.
Notes:

1. A chain polymerization consists of initiation and propagation reactions, and may also include termination and chain transfer reactions.
2. The adjective 'chain' in 'chain polymerization' denotes a 'chain reaction' rather than a 'polymer chain'.
3. Propagation in chain polymerization usually occurs without the formation of small molecules. However, cases exist where a low-molar-mass by-product is formed, as in the polymerization of oxazolidine-2,5-diones derived from amino acids (commonly termed amino-acid *N*-carboxy anhydrides). When a low-molar-mass by-product is formed, the adjective 'condensative' is recommended to give the term condensative chain polymerization
4. The growth steps are expressed by:

   $$\mathrm{P}_x + \mathrm{M} \rightarrow \mathrm{P}_{x+1}\ (+\mathrm{L}) \qquad \{x\} \in \{1, 2, \ldots\infty\}$$

   where P_x denotes the growing chain of degree of polymerization x, M a monomer and L a low-molar-mass by-product formed in the case of condensative chain polymerization.
5. The term 'chain polymerization' may be qualified further, if necessary, to specify the type of chemical reactions involved in the growth step, e.g. ring-opening chain polymerization, cationic chain polymerization.

6. There exist, exceptionally, some polymerizations that proceed *via* chain reactions that, according to the definition, are not chain polymerizations. For example, the polymerization:



proceeds *via* a radical chain reaction with intermolecular transfer of the radical centre. The growth step, however, involves reactions between molecules of all degrees of polymerization and, hence, the polymerization is classified as a polyaddition. If required, the classification can be made more precise and the polymerization described as a chain-reaction polyaddition.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2306

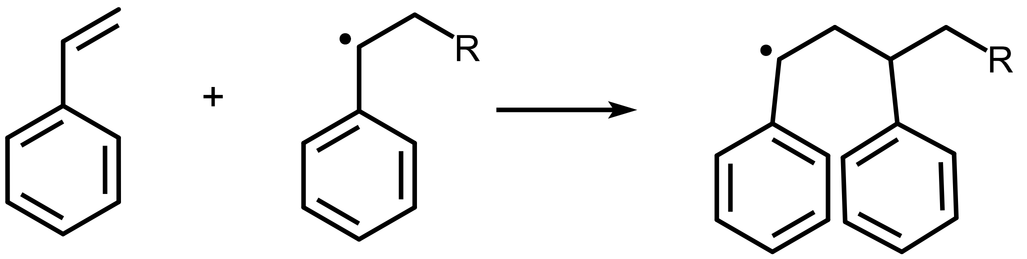
chain reaction

A reaction in which one or more reactive reaction intermediates (frequently radicals) are continuously regenerated, usually through a repetitive cycle of elementary steps (the 'propagation step'). For example, in the chlorination of methane by a radical mechanism, $Cl^{\cdot}$ is continuously regenerated in the chain propagation steps:

$$Cl^{\bullet} + CH_4 \longrightarrow HCl + H_3C^{\bullet} \qquad \text{Propagation steps}$$

$$H_3C^{\bullet} + Cl_2 \longrightarrow CH_3Cl + Cl^{\bullet}$$

In chain polymerization reactions, reactive intermediates of the same types, generated in successive steps or cycles of steps, differ in relative molecular mass, as in:



See also: chain branching, chain transfer, degenerate chain branching, initiation, termination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1094
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2293
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 157

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2179

chain scission

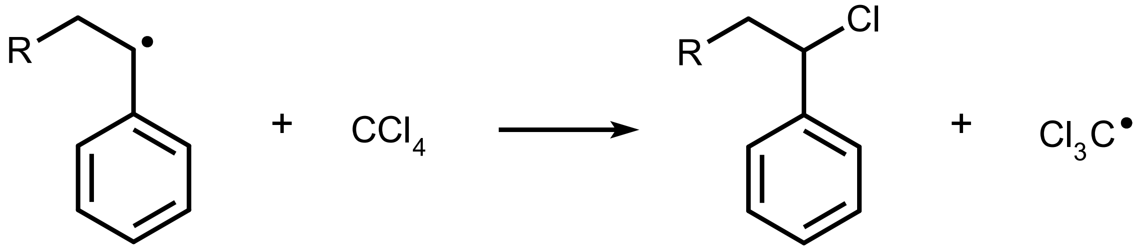
of a polymer

A chemical reaction resulting in the breaking of skeletal bonds.

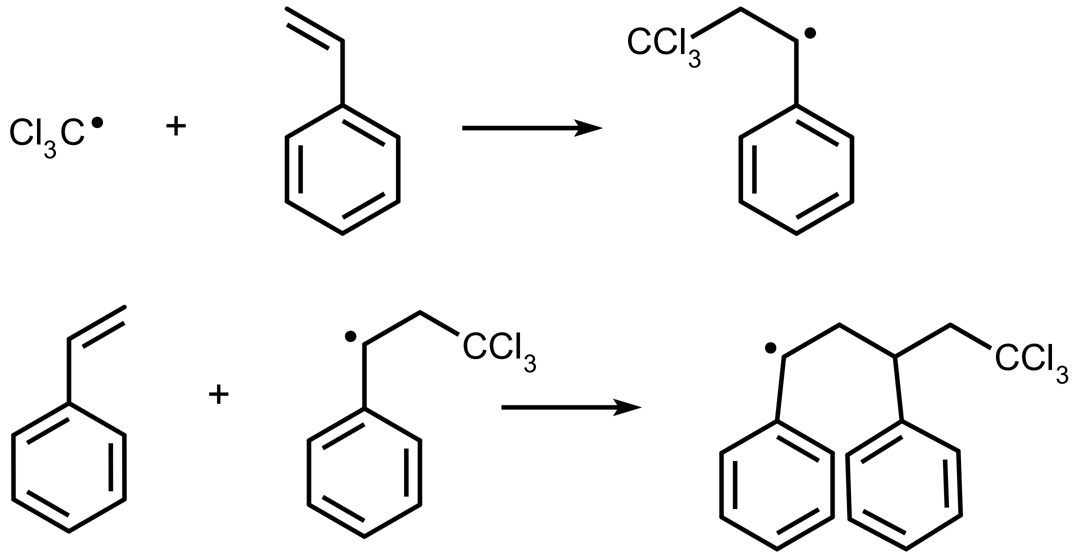
Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2309

chain transfer

The abstraction, by the radical end of a growing chain-polymer, of an atom from another molecule. The growth of the polymer chain is thereby terminated but a new radical, capable of chain propagation and polymerization, is simultaneously created. For the example of alkene polymerization cited for a chain reaction, the reaction:



represents a chain transfer, the radical $Cl_3C^{\cdot}$ inducing further polymerization:



The phenomenon occurs also in other chain reactions such as cationic polymerization.
See also: telomerization

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1094

chain-ending step

See: initiation

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 762

chain-orientational disorder

in polymer crystals

Structural disorder resulting from the statistical coexistence within the crystals of identical chains with opposite orientations. A typical example is provided by the up-down statistical coexistence of anticlined chains in the same crystal structure.

Source:
Purple Book, p. 80

chain-propagating reaction

Synonym: propagating reaction

A chain-propagating reaction, or more simply a propagating reaction, is an elementary step in a chain reaction in which one chain carrier is converted into another. The conversion can be a unimolecular reaction or a bimolecular reaction with a reactant molecule.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 157

chain-termination reaction

See: termination

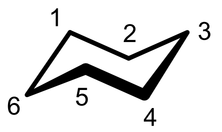
Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 157
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1173

chair, boat, twist

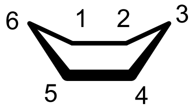
Also contains definition of: twist form

If carbon atoms 1, 2, 4 and 5 of cyclohexane occupy coplanar positions and when carbon atoms 3 and 6 are on opposite sides of the plane the conformation (of symmetry group D_{3d}) is called a chair form. The

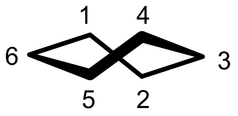
same term is applied to similar conformations of analogous saturated six-membered ring structures containing hetero-atoms and/or bearing substituent groups, but these conformations may be distorted from the exact D_{3d} symmetry. For cyclohexane and most such analogues, the chair form is the most stable conformation. If the cyclohexane conformation has no centre of symmetry but possesses two planes of symmetry, one of them bisecting the bonds between atoms 1 and 2 and between 4 and 5 and the other plane passing through atoms 3 and 6 (which lie out of the plane and on the same side of the plane containing 1, 2, 4 and 5), that conformation (of symmetry group C_{2v}) is called a boat form and it is generally not a stable form. Again, this term is also applied to structural analogues. The conformation of D_2 symmetry passed through in the interconversion of two boat forms of cyclohexane is called the twist form (also known as skew boat, skew form and stretched form).
See also: half-chair



chair (D_{3d})



boat (C_{2v})



twist (D_2)

In a five-membered ring a conformation in which two adjacent atoms are maximally displaced, in opposite directions, relative to the plane containing the other three carbon atoms has been called a half-chair but is better called a twist conformation.
See also: envelope conformation
In carbohydrate chemistry the term twist refers to a five-membered ring and the D_2 symmetry six-membered ring is referred to as skew.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2202

chair–chair interconversion

See: ring reversal

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2202

chalcones

1,3-Diphenylpropenone (benzylideneacetophenone), ArCH=CH(=O)Ar, and its derivatives formed by substitution.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1327

chamber saturation

in gas chromatography

Uniform distribution of the eluent vapour throughout the chamber prior to chromatography.

Source:
Orange Book, p. 99

change of a quantity

The increment of the value of a quantity Q with time. The change may be expressed either infinitesimally at time t by the differential $\mathrm{d}Q$ or $\mathrm{d}Q(t)$, or in practice it may be expressed by a finite increment over the time interval $(t_1;\, t_2)$, i.e. $Q(t_2) - Q(t_1)$, which may be written ΔQ or $\Delta Q(t_1;\, t_2)$

$$\Delta Q = \Delta Q(t_1;\, t_2) = Q(t_2) - Q(t_1)$$

Examples are: mass change, Δm; amount of substance change, Δn; volume change, ΔV; substance concentration change, Δc.

Source:
PAC, 1992, *64*, 1569 *(Quantities and units for metabolic processes as a function of time (IUPAC Recommendations 1992))* on page 1571

change ratio of a quantity

A term which may be expressed infinitesimally at time t by a ratio of differentials $\frac{\mathrm{d}Q_1(t)}{\mathrm{d}Q_2(t)}$ where the kind of quantities are the same but for different components in the same system. In practice, the ratio for a finite interval is:

$$\frac{\Delta Q_1(t_1;\, t_2)}{\Delta Q_2(t_1;\, t_2)}$$

Examples are: mass change ratio, $\frac{\mathrm{d}m_1(t)}{\mathrm{d}m_2(t)}$; amount of substance change ratio, $\frac{\mathrm{d}n_1(t)}{\mathrm{d}n_2(t)}$.

Source:
PAC, 1992, *64*, 1569 *(Quantities and units for metabolic processes as a function of time (IUPAC Recommendations 1992))* on page 1571

channel

1. Regions of potential-energy surfaces where there are valleys are sometimes referred to as arrangement channels. The reactant channel or entrance channel is that corresponding to configurations similar to those of the reactants; the product channel or exit channel relates to configurations similar to those of the products. In collision theory, the specification of a complete set of quantum numbers in a given arrangement channel is called a channel.
   See also: entrance channel, exit channel

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 157

2. (*in analysis*) That part of an analytical instrument that is dedicated to a single analytical procedure, including the transducer. This term relates to the internal operation of certain types of instruments, particularly in clinical chemistry. The general term channel has a much broader meaning, and the term is not recommended.

   Source:
   PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

chaperon

A species that facilitates a combination reaction between atoms or radicals, or the reverse process, is known as a chaperon. It is a special case of a third body.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 157

char

A solid decompostion product of a natural or synthetic organic material.
Note:
If the precursor has not passed through a fluid stage, char will retain the characteristic shape of the precursor (although becoming of smaller size). For such materials the term 'pseudomorphous' has been used. Some simple organic compounds, e.g. sugar, melt at an early stage of decomposition and then polymerize during carbonization to produce chars.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 484

characteristic group

in organic nomenclature

A single heteroatom, for example, –Cl and =O; a heteroatom bearing one or more hydrogen atoms or other heteroatoms, for example, $-NH_2$, –OH, $-SO_3H$, $-PO_3H_2$ and IO_2 ; or a heteroatomic group attached to or containing a single carbon atom, for example, –CHO, –C≡N, –COOH and –NCO , attached to a parent hydride.

Source:
Blue Book (Guide), p. 13

characteristic

in analytical chemistry

A property or attribute of a material that is measured, compared or noted. Attributes are ordinarily qualitative characteristics, but quantitative characteristics (variables) may be converted into attributes by assigning items to certain categories on the basis of the measured values. The value of the characteristic determined as a result of an observation or test is the observed value; when determined by a specified test method, it is called the test result. The concentration or quantity of an analyte as estimated by use of a sample is usually the characteristic of interest in analytical chemistry.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1201

characteristic length

Synonym: characteristic scale *in thin films*

in thin films

The term characteristic length or scale refers, in general, to the parameter which characterizes the density profile (of a given physical quantity). The static (equilibrium) or dynamic character of a characteristic length must be specified. The terms out of plane and in plane refer to characteristic lengths normal or parallel to the interface, respectively. Since interfacial layer 'thickness' and characteristic length correspond to various concepts, the current usage where an out of plane characteristic length is referred to as the interfacial layer thickness, is confusing and should be abandoned.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1674

characteristic mass for integrated absorbance, m_0

in electrothermal atomization

That mass of analyte which produces an integrated absorbance signal whose net area is equal to $0.0044\ \mathrm{s}$.

Source:
PAC, 1992, *64*, 253 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XII. Terms related to electrothermal atomization (IUPAC Recommendations 1992))* on page 258

characteristic mass for peak absorption, m_p

in electrothermal atomization

That mass of analyte which produces a defined peak absorbance of 0.0044 (or 1% absorbance).

Source:
PAC, 1992, *64*, 253 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XII. Terms related to electrothermal atomization (IUPAC Recommendations 1992))* on page 258

characteristic mass, m_c

in electrothermal atomization

The mass of analyte which, when atomized electrothermally, produces the uniquely defined absorption signal.

Source:
PAC, 1992, *64*, 253 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XII. Terms related to electrothermal atomization (IUPAC Recommendations 1992))* on page 258

characteristic potential

An applied potential that is characteristic of a charge-transfer process and the experimental conditions (such as the composition of the solvent and supporting electrolyte and the temperature) under which it is investigated, and whose nature depends on the technique that is employed. Some typical characteristic potentials are the half-wave potential in polarography, the quarter-transition-time potential in chronopotentiometry, the peak potential and the half-peak potential in linear-sweep voltammetry, and the summit potential in ac polarography.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1493

characteristic ratio

in polymers

The ratio of the mean-square end-to-end distance, $< r^2 >_0$, of a linear polymer chain in a theta state to $N{\cdot}L^2$, where N is the number of rigid sections in the main chain, each of length L; if all of the rigid sections are not of equal length, the mean-square value of L is used, i.e.

$$L^2 = \sum_i \frac{L_i^{\bar{2}}}{N}$$

In simple single-strand chains, the bonds are taken as the rigid sections. The recommended symbol is: C_N (C_∞ when $N \rightarrow \infty$).

Source:
Purple Book, p. 49

characteristic X-ray emission

Also contains definitions of: fluorescence excitation
of X-rays

, primary excitation

of X-rays

, secondary excitation
of X-rays

Synonym: characteristic X-radiation

X-ray emission originates from the radiative decay of electronically highly excited states of matter. Excitation by electrons is called primary excitation and by photons, secondary or fluorescence excitation. Particle induced X-ray emission (PIXE) is produced by the excitation of heavier particles such as protons, deuterons or heavy atoms in varying degrees of ionization. Emission of photons in the X-ray wavelength region also occurs from ionized gases or plasmas at high temperatures, from nuclear processes (low-energy end of the gamma-ray spectrum) and from radiative transitions between muonic states. Characteristic X-ray emission consists of a series of X-ray spectral lines with discrete frequencies, characteristic of the emitting atom. Other features are emission bands from transitions to valence levels. In a spectrum obtained with electron or photon excitation the most intense lines are called diagram lines or normal X-ray lines. They are dipole allowed transitions between normal X-ray diagram levels.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 737

charcoal

A traditional term for a char obtained from wood, peat, coal or some related natural organic materials.
Note:
Charcoal has highly reactive inner surfaces and a low sulfur content. It has or has had, therefore, a variety of uses, e.g. in ferrous metallurgy and for gunpowder (minor uses: medical purposes and paint materials).

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 484

charge

See: electric charge, elementary charge

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 965

charge density, ρ

Electric charge divided by the volume it occupies.
See also: electron density

Source:
Green Book, 2nd ed., p. 14

charge hopping

Electron or hole transfer between equivalent sites.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2231

charge number, z

Ratio of the charge of a particle to the elementary charge.

Source:
Green Book, 2nd ed., p. 44
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 965
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1544

charge number

in inorganic nomenclature

The magnitude of the charge on an ion, given in arabic numerals followed by the sign of the charge, in parentheses without a space, immediately after the name of an ion, e.g. iron(2+), hexacyanoferrate(4−).
Note:
The term Ewens–Bassett number is no longer recommended.

Source:
Red Book, p. 66

charge number n, ν_e, z

of a cell reaction

Number of electrons transferred according to the cell reaction equation.

Source:
Green Book, 2nd ed., p. 58

charge population

The net electric charge on a specified atom in a molecular entity, as determined by some prescribed definition.
See also: electron density

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1094

charge recombination

Reverse of charge separation. In using this term it is important to specify the resulting electronic state of the donor and acceptor.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2231

charge separation

A process in which, under the influence of a suitable driving force (e.g. provided by photoexcitation), electronic charge moves in a direction that increases the difference in local charges between donor and acceptor sites. Electron transfer between neutral species is one of the most important examples.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2231

charge shift

A process in which under the influence of a suitable driving force (e.g. provided by photoexcitation) electronic charge moves without changing the difference in local charges between donor and acceptor sites. Electron transfer reversing the charges in a system composed of a neutral donor and a cationic acceptor or of a neutral acceptor and an anionic donor provide prominent examples.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2231

charge transfer transition to solvent (CTTS)

Electronic transition which is adequately described by single electron transfer between a solute and the solvent, as opposed to excitation followed by electron transfer to solvent.
See also: charge-transfer transition

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232

charge-exchange ionization

in mass spectrometry

This occurs when an ion/atom or ion/molecule reaction takes place in which the charge on the ion is transferred to the neutral species without any dissociation of either. Synonymous with charge-transfer ionization.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

charge-exchange reaction

Synonymous with charge-transfer reaction.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

charge-inversion mass spectrum

Charge inversion processes of the types:

$$M^{+} + X \longrightarrow M^{-} + X^{2+}$$

or

$$M^{-} + X \longrightarrow M^{+} + X + 2e^{-}$$

respectively, occuring in a collision cell (containing a gas, X) located in a field-free region preceding a magnetic and electric sector combination placed in either order, may be detected as follows. If the instrument slits are wide, and if the connections to the two sectors, appropriate to transmission of either positive or negative main-beam ions, are simply reversed, the negative or positive product ions of the two processes, respectively, will be transmitted. If the magnetic field is scanned, a spectrum of such product ions will be obtained, and this spectrum is called a charge-inversion mass spectrum. These spectra are sometimes referred to as $-E$ and $+E$ spectra, respectively. The terms '$2E$, $E/2$, $-E$ or $+E$ mass spectrum' should not be used without prior explanation of the meaning $2E$, E, $+E$ or $-E$.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1551

charge-permutation reaction

A general term to describe an ion/neutral species reaction where there is a change in the magnitude and/or sign of the charges of the reactant.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

charge-stripping reaction

An ion/neutral species reaction wherein the charge on the reactant ion is made more positive.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

charge-transfer adsorption

Oxidative or reductive chemisorption where 'reductive' and 'oxidative' refer to electron gain or loss on species in the solid. In simple cases it is non-dissociative, i.e. there is a mere transfer of charge between adsorptive and adsorbent in forming the adsorbate.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

charge-transfer complex

An electron-donor–electron-acceptor complex, characterized by electronic transition(s) to an excited state in which there is a partial transfer of electronic charge from the donor to the acceptor moiety.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1094

charge-transfer (CT) state

A state related to the ground state by a charge-transfer transition.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232

charge-transfer (CT) transition

An electronic transition in which a large fraction of an electronic charge is transferred from one region of a molecular entity, called the electron donor, to another, called the electron acceptor (intramolecular CT) or from one molecular entity to another (intermolecular CT). Typical for donor-acceptor complexes or multichromophoric molecular entities. In some cases the charge-transfer absorption band may be obscured by the absorption of the partners.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232

charge-transfer device

in radiation detection

A charge-transfer device has a metal oxide semiconductor (MOS) structure that is composed of many independent pixels where charge is stored in such a way that the charge pattern corresponds to the irradiation pattern. These devices can be linear or two-dimensional. According to the method used to detect the charge pattern, two types of charge-transfer devices can be distinguished: charge-coupled devices (CCDs) and charge-injection devices (CIDs).

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1757

charge-transfer reaction

in mass spectrometry

An ion/neutral species reaction wherein the total charge on the reactant ion is transferred initially to the reactant neutral species so that the reactant ion becomes a neutral entity. Considering some of the possible reactions of ions M^{2+}, M^{+} and M^{-} with a neutral species X, these would be further categorized as follows:

$$M^{2+} + X \longrightarrow M^{+} + X^{+}$$

(Partial charge transfer)

$$M^{+} + X \longrightarrow M^{2+} + X + e^{-}$$

(Charge stripping)

$$M^{-} + X \longrightarrow M^{+} + X + 2e^{-}$$

(Charge stripping and charge inversion)

All are ion/neutral species reactions and also charge permutation reactions.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

charge-transfer step

of an electrode reaction

An elementary step in which charge is transferred from one phase to the other.

Source:
PAC, 1980, *52*, 233 *(Electrode reaction orders, transfer coefficients and rate constants. Amplification of definitions and recommendations for publication of parameters)* on page 235

charring

Pyrolysis of samples containing organic matter. In the presence of oxygen this is referred to as ashing.

Source:
PAC, 1992, *64*, 253 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XII. Terms related to electrothermal atomization (IUPAC Recommendations 1992))* on page 256

chelate

See: chelation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1094
Red Book, p. 147

chelating polymer

Polymer containing ligand groups capable of forming bonds (or other attractive interactions) between two or more separate binding sites within the same ligand group and a single atom.
Notes:
1. Chelating polymers mostly act as ion-exchange polymers specific to ions that form chelates with chelating ligands of the polymer.
2. ***See also:*** chelation.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 895

chelation

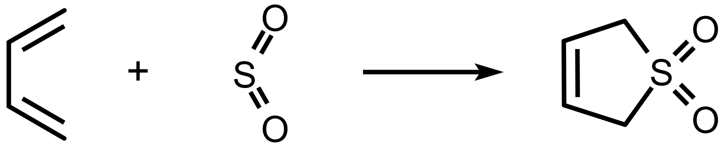
The formation or presence of bonds (or other attractive interactions) between two or more separate binding sites within the same ligand and a single central atom. A molecular entity in which there is chelation (and the corresponding chemical species) is called a 'chelate'. The terms bidentate (or didentate), tridentate, tetradentate, ... multidentate are used to indicate the number of potential binding sites of the ligand, at least two of which must be used by the ligand in forming a 'chelate'. For example, the bidentate ethylenediamine forms a chelate with CuI in which both nitrogen atoms of ethylenediamine are bonded to copper. (The use of the term is often restricted to metallic central atoms.) The phrase 'separate binding sites' is intended to exclude cases such as $[PtCl_3(CH_2{=}CH_2)]^-$, ferrocene and (benzene)tricarbonylchromium in which ethene, the cyclopentadienyl group and benzene, respectively, are considered to present single binding sites to the respective metal atom, and which are not normally thought of as chelates.

See also: cryptand, η (eta or hapto)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1094
Red Book, p. 147

cheletropic reaction

A form of cycloaddition across the terminal atoms of a fully conjugated system with formation of two new σ-bonds to a single atom of the ('monocentric') reagent. There is formal loss of one π-bond in the substrate and an increase in coordination number of the relevant atom of the reagent. An example is the addition of sulfur dioxide to butadiene:



The reverse of this type of reaction is designated 'cheletropic elimination'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1094

chelotropic reaction

Alternative (and etymologically more correct) name for cheletropic reaction.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1095

chemi-ionization

in mass spectrometry

This refers to a process whereby gaseous molecules are ionized when they interact with other internally excited gaseous molecules or molecular moieties. Chemi-ionization and chemical ionization are two terms which should not be used interchangeably.
See also: associative ionization, chemical ionization

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547
Orange Book, p. 204

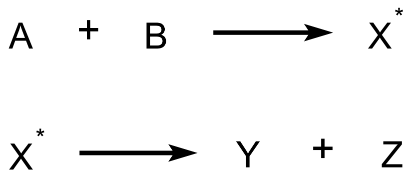
chemical actinometer

A detector in which the amount of a chemical formed is proportional to the numbers of photons absorbed.
See also: actinometer

Source:
Orange Book, p. 193

chemical activation

When some of the energy required for a reaction is provided by a preceding exothermic chemical reaction there is said to be chemical activation. For example, in the scheme:



$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{X}^*$$

$$\mathrm{X}^* \longrightarrow \mathrm{Y} + \mathrm{Z}$$

some or all of the energy required for X to decompose is provided by the first reaction.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 158

chemical amount

See: amount of substance

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 965
Green Book, 2nd ed., p. 46

chemical amplification

Process consisting of a chemical reaction that generates a species that catalyzes another reaction and also the succeeding catalyzed reaction.
Notes:

1. Chemical amplification can lead to a change in structure and by consequence to a change in the physical properties of a polymeric material.
2. The term 'chemical amplification' is commonly used in photo-resist lithography employing a photo-acid generator or photo-base generator.
3. An example of chemical amplification is the transformation of [(*tert*-butoxycarbonyl)oxy]phenyl groups in polymer chains to hydroxyphenyl groups catalyzed by a photo-generated acid.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 891

chemical bond

When forces acting between two atoms or groups of atoms lead to the formation of a stable independent molecular entity, a chemical bond is considered to exist between these atoms or groups. The principal characteristic of a bond in a molecule is the existence of a region between the nuclei of constant potential contours that allows the potential energy to improve substantially by atomic contraction at the expense of only a small increase in kinetic energy. Not only directed covalent bonds characteristic of organic compounds, but also bonds such as those existing between sodium cations and chloride anions in a crystal of sodium chloride or the bonds binding aluminium to six molecules of water in its environment, and even weak bonds that link two molecules of O_2 into O_4, are to be attributed to chemical bonds.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1930

chemical decomposition

The breakdown of a single entity (normal molecule, reaction intermediate, etc.) into two or more fragments.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1104

chemical diffusion

Diffusion under the influence of a gradient in chemical composition. In concentrated solid solutions, e.g. $A_{1-x}B_x$, or in diffusion couples, the motion of one constituent causes a counterflow of the other constituents(s) or vacancies. In this case one can define a diffusion coefficient for the intermixing, which is called the chemical diffusion coefficient or interdiffusion coefficient.

Source:
PAC, 1999, *71*, 1307 *(Definitions of Terms for Diffusion in the Solid State)* on page 1310

chemical dosimeter

A dosimeter in which the dose is measured by observing the extent, under specified conditions, of a chemical reaction caused by the ionizing radiation to be measured.

Source:
Orange Book, p. 215

chemical element

1. A species of atoms; all atoms with the same number of protons in the atomic nucleus.
2. A pure chemical substance composed of atoms with the same number of protons in the atomic nucleus. Sometimes this concept is called the elementary substance as distinct from the chemical element as defined under 1, but mostly the term chemical element is used for both concepts.

Source:
Physical Chemistry Division, unpublished
Red Book, p. 35

chemical equilibrium

Reversible processes [processes which may be made to proceed in the forward or reverse direction by the (infinitesimal) change of one variable], ultimately reach a point where the rates in both directions are identical, so that the system gives the appearance of having a static composition at which the Gibbs energy, G, is a minimum. At equilibrium the sum of the chemical potentials of the reactants equals that of the products, so that:

$$\Delta G_{\mathrm{r}} = \Delta G_{\mathrm{r}}^{\mathrm{o}} + R\,T \ln K = 0$$

$$\Delta G_{\mathrm{r}}^{\mathrm{o}} = -R\,T \ln K$$

The equilibrium constant, K, is given by the mass-law effect.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1114

chemical flux, φ

A concept related to rate of reaction, particularly applicable to the progress in one direction only of component reaction steps in a complex system or to the progress in one direction of reactions in a system at dynamic equilibrium (in which there are no observable concentration changes with time). Chemical flux is a derivative with respect to time, and has the dimensions of amount of substance per unit volume transformed per unit time. The sum of all the chemical fluxes leading to destruction of B is designated the 'total chemical flux out of B' (symbol $\sum \varphi_{-\mathrm{B}}$); the corresponding formation of B by concurrent elementary reactions is the 'total chemical flux into B or A' (symbol $\sum \varphi_{\mathrm{B}}$). For the mechanism:

$$\mathrm{A} + \mathrm{B} \underset{-1}{\overset{1}{\rightleftharpoons}} \mathrm{C}$$

$$\mathrm{C} + \mathrm{D} \overset{2}{\rightleftharpoons} \mathrm{E}$$

the total chemical flux into C is caused by the single reaction (1):

$$\sum \varphi_{\mathrm{C}} = \varphi_1$$

whereas the chemical flux out of C is a sum over all reactions that remove C:

$$\sum \varphi_{-\mathrm{C}} = \varphi_{-1} + \varphi_2$$

where φ_{-1} is the 'chemical flux out of C into B (and/or A)' and φ_2 is the 'chemical flux out of C into E'. The rate of appearance of C is then given by:

$$\frac{\mathrm{d}[\mathrm{C}]}{\mathrm{d}t} = \sum \varphi_{\mathrm{C}} - \sum \varphi_{-\mathrm{C}}$$

In this system φ_1 (or $\sum \varphi_{-\mathrm{A}}$) can be regarded as the hypothetical rate of decrease in the concentration of A due to the single (unidirectional) reaction (1) proceeding in the assumed absence of all other reactions. For a non-reversible reaction:

$$\mathrm{A} \xrightarrow{1} \mathrm{P}$$

$$-\frac{\mathrm{d}[\mathrm{A}]}{\mathrm{d}t} = \varphi_1$$

If two substances A and P are in chemical equilibrium:

$$\mathrm{A} \rightleftarrows \mathrm{P}$$

then:

$$\sum \varphi_{\mathrm{A}} = \sum \varphi_{-\mathrm{A}} = \sum \varphi_{\mathrm{P}} = \sum \varphi_{-\mathrm{P}}$$

and

$$-\frac{\mathrm{d}[\mathrm{A}]}{\mathrm{d}t} = \frac{\mathrm{d}[\mathrm{P}]}{\mathrm{d}t} = 0$$

See also: order of reaction, rate-limiting step, steady state

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1095

chemical functionality

Ability of functional groups present within a polymer or polymer network to participate in chemical reactions.
Note:
The chemical functionality of a network formed by a sol-gel process from a precursor such as $(RO)_3Si–CH=CH_2$ is that of the vinyl group.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1804

chemical induction (coupling)

When in a chemical system one reaction accelerates another there is said to be chemical induction or coupling. It is due to an intermediate or product of the inducing reaction participating in the second reaction. Chemical induction is often observed in oxidation–reduction reactions, chain reactions, and biological reactions. Sometimes a reaction having $\Delta G^{\mathrm{o}} > 0$ is induced by a simultaneous process having $\Delta G^{\mathrm{o}} < 0$.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 158

chemical ionization

in mass spectrometry

This concerns the process whereby new ionization species are formed when gaseous molecules interact with ions. The process may involve transfer of an electron, proton or other charged species between the reactants. When a positive ion results from chemical ionization, the term may be used without qualification. When a negative ion is involved, the term negative ion chemical ionization should be used; note that negative ion formation by attachment of a free electron does not fall within this definition. Chemical ionization and chemi-ionization are two terms which should not be used interchangeably.
See: electron attachment
See also: chemi-ionization

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547
Orange Book, p. 204
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2179

chemical isotope exchange

Exchange of isotopes between different types of molecules or ions in the course of a chemical reaction.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

chemical laser

A continuous wave or pulsed laser in which the excitation and population inversion of the emitting species result from a chemical reaction. Typical examples are HF and DF lasers emitting many lines in the IR region.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232

chemical measurement process (CMP)

An analytical method of defined structure that has been brought into a state of statistical control, such that its imprecision and bias are fixed, given the measurement conditions. This is prerequisite for the evaluation of the performing characteristics of the method, or the development of meaningful uncertainty statements concerning analytical results.

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1702

chemical modification

Process by which at least one feature of the chemical constitution of a polymer is changed by chemical reaction(s).
Note:
A configurational change (*e.g.*, *cis–trans* isomerization) is not usually referred to as a chemical modification.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 891

chemical oxygen demand (COD)

A measure of the amount of oxygen, divided by the volume of the system, required to oxidize the organic (and inorganic) matter in wastewater using a chemically oxidizing agent. In practice, it is usually expressed in milligrams O_2 per litre.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 149

chemical potential, μ_B

The chemical potential of a substance **B** in a mixture of substances **B**, **C** ... is related to the Gibbs energy G of the mixture by:

$$\mu_{\mathrm{B}} = \left(\frac{\partial G}{\partial n_{\mathrm{B}}}\right)_{T,p,n_{\mathrm{C}\neq\mathrm{B}}}$$

where T is the thermodynamic temperature, p is the pressure and n_{B}, n_{C}, ... are the amounts of substance of **B**, **C**, ... For a pure substance **B**, the chemical potential μ_{B}^{*} is given by:

$$\mu_{\mathrm{B}}^{*} = \frac{G^{*}}{n_{\mathrm{B}}} = G_{\mathrm{m}}^{*}$$

where G_{m}^{*} is the molar Gibbs energy, and where the superscript * attached to a symbol denotes the property of the pure substance. The superscript $_{\ominus}$ or $_{\mathrm{o}}$ attached to a symbol may be used to denote a standard thermodynamic quantity.
See also: standard chemical potential

Source:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 535
Green Book, 2nd ed., p. 49
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 966

chemical reaction

A process that results in the interconversion of chemical species. Chemical reactions may be elementary reactions or stepwise reactions (It should be noted that this definition includes experimentally observable interconversions of conformers.) Detectable chemical reactions normally involve sets of molecular entities as indicated by this definition, but it is often conceptually convenient to use the term also for changes involving single molecular entities (i.e. 'microscopic chemical events').
See also: identity reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1096

chemical reaction equation

Symbolic representation of a chemical reaction where the reactant entities are given on the left hand side and the product entities on the right hand side. The coefficients next to the symbols and formulae of entities are the absolute values of the stoichiometric numbers. Different symbols are used to connect the reactants and products with the following meanings: $=$ for a stoichiometric relation; $\rightarrow$ for a net forward reaction; $\leftrightarrows$ for a reaction in both directions; $\leftrightharpoons$ for equilibrium.

Source:
Green Book, 2nd ed., p. 45

chemical relaxation

Also contains definition of: T-jump

If the equilibrium mixture of a chemical reaction is disturbed by a sudden change, especially of some external parameter (such as temperature, pressure or electrical field strength), the system will readjust itself to a new position of the chemical equilibrium or return to the original position, if the perturbation is temporary. The readjustment is known as chemical relaxation. In many cases, and in particular when the displacement from equilibrium is slight, the progress of the system towards equilibrium can be expressed as a first-order law:

$$C_t - (C_{\mathrm{eq}})_2 = \left[(C_{\mathrm{eq}})_1 - (C_{\mathrm{eq}})_2\right] \mathrm{e}^{\frac{-t}{\tau}}$$

where $(C_{\mathrm{eq}})_1$ and $(C_{\mathrm{eq}})_2$ are the equilibrium concentrations of one of the chemical species involved in the reaction before and after the change in the external parameter, and C_t is its concentration at time t. The time parameter τ, named relaxation time, is related to the rate constants of the chemical reaction involved. Measurements of the relaxation times by relaxation methods [involving a temperature jump (T-jump), pressure jump, electric field jump or a periodic disturbance of an external parameter, as in ultrasonic techniques] are commonly used to follow the kinetics of very fast reactions.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1096

chemical shift, δ

in NMR

The fractional variation of the resonance frequency of a nucleus in nuclear magnetic resonance (NMR) spectroscopy in consequence of its magnetic environment. The chemical shift of a nucleus, δ, is expressed as a ratio involving its frequency, ν_{cpd}, relative to that of a standard, ν_{ref}, and defined as:

$$\delta = \frac{\nu_{\mathrm{cpd}} - \nu_{\mathrm{ref}}}{\nu_{\mathrm{ref}}}$$

δ-values are normally expressed in ppm. For ^{1}H and ^{13}C NMR the reference signal is usually that of tetramethylsilane (TMS), strictly speaking in dilute solution in $CDCl_3$. Other references are used in the older literature and for other solvents, such as D_2O. Resonance lines to high frequency from the TMS signal have positive, and resonance lines to low frequency from TMS have negative, δ-values (arising from relative deshielding and shielding respectively). The archaic terms 'downfield' and 'upfield' should no longer be used. For nuclei other than ^{1}H, chemical shifts are expressed either in the same manner relative to an agreed substance containing the relevant nucleus or relative to the ^{1}H resonance of TMS as Ξ values, defined in the references below.

Source:
PAC, 2001, *73*, 1795 *(NMR nomenclature. Nuclear spin properties and conventions for chemical shifts (IUPAC Recommendations 2001))* on page 1807

PAC, 2008, *80*, 59 *(Further conventions for NMR shielding and chemical shifts (IUPAC Recommendations 2008))* on page 61
Green Book, 3rd ed., p. 29

chemical shift

in photoelectron and Auger spectra

The displacement of photoelectron or Auger peak energies originating from changes in electron binding energies as a consequence of differences in the chemical environment of the atoms.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

chemical species

An ensemble of chemically identical molecular entities that can explore the same set of molecular energy levels on the time scale of the experiment. The term is applied equally to a set of chemically identical atomic or molecular structural units in a solid array. For example, two conformational isomers may be interconverted sufficiently slowly to be detectable by separate NMR spectra and hence to be considered to be separate chemical species on a time scale governed by the radiofrequency of the spectrometer used. On the other hand, in a slow chemical reaction the same mixture of conformers may behave as a single chemical species, i.e. there is virtually complete equilibrium population of the total set of molecular energy levels belonging to the two conformers. Except where the context requires otherwise, the term is taken to refer to a set of molecular entities containing isotopes in their natural abundance. The wording of the definition given in the first paragraph is intended to embrace both cases such as graphite, sodium chloride or a surface oxide, where the basic structural units may not be capable of isolated existence, as well as those cases where they are. In common chemical usage generic and specific chemical names (such as radical or hydroxide ion) or chemical formulae refer either to a chemical species or to a molecular entity.
See also: chemical species (of an element)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1096
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2202

chemical species

of an element

Specific form of an element defined as to isotopic composition, electronic or oxidation state, and/or complex or molecular structure.
See also: chemical species

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1044

chemical substance

Matter of constant composition best characterized by the entities (molecules, formula units, atoms) it is composed of. Physical properties such as density, refractive index, electric conductivity, melting point etc. characterize the chemical substance.

Source:
Physical Chemistry Division, unpublished

chemical vapour generation

in spectrochemical analysis

A system in which the analyte is separated from the sample matrix by the generation of gaseous species as a result of a chemical reaction.

Source:
PAC, 1992, *64*, 261 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XIII. Terms related to chemical vapour generation (IUPAC Recommendations 1992))* on page 262

chemical yield

The fraction of the amount of an element or chemical compound following a specified chemical reaction or separation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

chemically bonded hybrid (material)

Hybrid material in which the different components are bonded to each other by covalent or partially covalent bonds.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1811

chemically induced dynamic electron polarization (CIDEP)

Non-Boltzmann electron spin- state population produced in thermal or photochemical reactions, either from a combination of radical pairs (called radical-pair mechanism), or directly from the triplet state (called triplet mechanism) and detectable by ESR spectroscopy.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 313

chemically initiated electron exchange luminescence (CIEEL)

Type of luminescence resulting from a thermal electron-transfer reaction. Also called catalyzed chemiluminescence.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 313

chemiexcitation

Generation, by a chemical reaction, of electronically excited molecular entities from reactants in their ground electronic states.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232

chemiflux

See: chemical flux

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1095

chemiluminescence

Emission of radiation resulting from a chemical reaction. The emitting species may be a reaction product or a species excited by energy transfer from an excited reaction product. The excitation may be electronic, vibrational or rotational; if the luminescence occurs in the infrared the expression infrared chemiluminescence is used.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 158
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 234

chemiluminescence analyser

An instrument consisting of a reaction chamber with separate inlets for the sample and reagent gas, an optical filter, a photomultiplier and a signal processing device. The reactive gas is introduced in excess. The quantity of light produced is proportional to the sample flow rate and the concentration of the measured substance in the sample under specified temperature and pressure conditions. The filter limits the wavelength to the region of interest and helps to eliminate interferences.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2179

chemiluminescent methods of detection

in analysis

Methods which utilize gas or liquid phase reactions between two molecules which produce a third molecule in an excited state. The wavelength distribution of the light emission from the excited molecule is characteristic of the species; in some circumstances this may be used to identify and to determine the concentration of one of the reacting species.

Source:
PAC, 1990, *62*, 17 *(Free energies of cation-molecule complex formation and cation-solvent transfers)* on page 21

chemisorption (chemical adsorption)

Adsorption which results from chemical bond formation (strong interaction) between the adsorbent and the adsorbate in a monolayer on the surface.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2179

chemometrics

Chemometrics is the application of statistics to the analysis of chemical data (from organic, analytical or medicinal chemistry) and design of chemical experiments and simulations.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1140

chemoselectivity (chemoselective)

Chemoselectivity is the preferential reaction of a chemical reagent with one of two or more different functional groups. A reagent has a high chemoselectivity if reaction occurs with only a limited number of different functional groups. For example, sodium tetrahydroborate is a more chemoselective reducing agent than is lithium tetrahydroaluminate. The concept has not been defined in more

quantitative terms. The term is also applied to reacting molecules or intermediates which exhibit selectivity towards chemically different reagents. Some authors use the term chemospecificity for 100% chemoselectivity. However, this usage is discouraged.
See also: regioselectivity, stereoselectivity, stereospecificity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1097

chemospecificity [obsolete]

See: chemoselectivity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1097

chemostat

A bioreactor in which constant growth conditions for microorganisms are maintained over prolonged periods of time by supplying the reactor with a continuous input of nutrients and continuous removal of medium.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 149

chimney effect

in atmospheric chemistry

A vertical movement of a localized mass of air or other gases which occurs due to local temperature differences.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2179

chiral

Having the property of chirality. As applied to a molecule the term has been used differently by different workers. Some apply it exclusively to the whole molecule, whereas others apply it to parts of a molecule. For example, according to the latter view, a *meso*-compound is considered to be composed of two chiral parts of opposite chirality sense; this usage is to be discouraged.
See: enantiomorph
In its application to an assembly of molecules, some restrict the term to an assembly in which all of the molecules have the same chirality sense, which is better called enantiopure. Others extend it to a racemic assembly, which is better just called a racemate. Use of the term to describe molecular assemblies should be avoided.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2202

chiral mobile phase

A mobile phase containing a chiral selector.

Source:
PAC, 1997, *69*, 1469 *(Analytical chiral separation methods (IUPAC Recommendations 1997))* on page 1472

chiral selector

The chiral component of the separation system capable of interacting enantioselectively with the enantiomers to be separated.

Source:
PAC, 1997, *69*, 1469 *(Analytical chiral separation methods (IUPAC Recommendations 1997))* on page 1472

chiral stationary phase

in liquid chromatography

A stationary phase which incorporates a chiral selector. If not a constituent of the stationary phase as a whole, the chiral selector can be chemically bonded to (chiral bonded stationary phase) or immobilised onto the surface of a solid support or column wall (chiral coated stationary phase), or simply dissolved in the liquid stationary phase.

Source:
PAC, 1997, *69*, 1475 *(Classification and characterization of stationary phases for liquid chromatography: Part I. Descriptive terminology (IUPAC Recommendations 1997))* on page 1479

chirality

The geometric property of a rigid object (or spatial arrangement of points or atoms) of being non-superposable on its mirror image; such an object has no symmetry elements of the second kind (a mirror plane, $\sigma = S_1$, a centre of inversion, $i = S_2$, a rotation-reflection axis, $S_{2\mathrm{n}}$). If the object is superposable on its mirror image the object is described as being achiral.
See also: handedness, superposability

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203
Blue Book, p. 479

chirality axis

Synonym: axis of chirality

An axis about which a set of ligands is held so that it results in a spatial arrangement which is not superposable on its mirror image. For example with an allene abC=C=Ccd the chiral axis is defined by the C=C=C bonds; and with an *ortho*-substituted biphenyl the atoms C-1, C-1', C-4 and C-4' lie on the chiral axis.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203

chirality centre

Synonym: centre of chirality

An atom holding a set of ligands in a spatial arrangement which is not superposable on its mirror image. A chirality centre is thus a generalized extension of the concept of the asymmetric carbon atom to central atoms of any element, for example N^+abcd, Pabc as well as Cabcd.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203

chirality element

Synonym: element of chirality

General name for a chirality axis, chirality centre or chirality plane. Also referred to as an element of chirality.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203

chirality plane

A planar unit connected to an adjacent part of the structure by a bond which results in restricted torsion so that the plane cannot lie in a symmetry plane. For example with (*E*)-cyclooctene the chiral plane includes the double bond carbon atoms and all four atoms attached to the double bond; with a monosubstituted paracyclophane the chiral plane includes the monosubstituted benzene ring with its three hydrogen atoms and the three other atoms linked to the ring (i.e. from the substituent and the two chains linking the two benzene rings).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203

chirality sense

The property that distinguishes enantiomorphs. The specification of two enantiomorphic forms by reference to an oriented space e.g. of a screw, a right threaded one or a left threaded one. The expression 'opposite chirality' is short for 'opposite chirality sense'.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203

chiroptic/chiroptical

A term referring to the optical techniques (using refraction, absorption or emission of anisotropic radiation) for investigating chiral substances [e.g. measurements of optical rotation at a fixed wavelength, optical rotatory dispersion (ORD), circular dichroism (CD), and circular polarization of luminescence (CPL)].

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203

chirotopic

Also contains definition of: achirotopic

The description of an atom (or point, group, face, etc. in a molecular model) that resides within a chiral environment. One that resides within an achiral environment has been called achirotopic.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203

chloramines

Amines substituted at nitrogen with one or two chlorine atoms (a contracted form of *N*-chloroamines).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328

chlorocarbons

Compounds consisting wholly of chlorine and carbon.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328

chlorohydrins

See: halohydrins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328

chromatogram

A graphical or other presentation of detector response, concentration of analyte in the effluent or other quantity used as a measure of effluent concentration versus effluent volume or time. In planar chromatography 'chromatogram' may refer to the paper or layer with the separated zones.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 823
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2179

chromatograph (noun)

The assembly of apparatus for carrying out chromatographic separation.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 823

chromatograph (verb)

To separate by chromatography.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 823

chromatographic detector

A device that measures the change of composition of the effluent.

Source:
Orange Book, p. 99
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 829

chromatography

A physical method of separation in which the components to be separated are distributed between two phases, one of which is stationary (stationary phase) while the other (the mobile phase) moves in a definite direction.
See also: adsorption chromatography, affinity chromatography, column chromatography, displacement chromatography, elution chromatography, exclusion chromatography, frontal chromatography, gas chromatography, ion-exchange chromatography, isothermal chromatography, liquid chromatography, normal-phase chromatography, partition chromatography, planar chromatography, programmed-flow chromatography (flow programming), programmed-pressure chromatography (pressure programming), programmed-temperature chromatography (temperature programming), pyrolysis-gas chromatography, reaction chromatography, reversed-phase chromatography, supercritical fluid chromatography, two-dimensional chromatography

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 823
Orange Book, p. 92
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2179

chromophore

The part (atom or group of atoms) of a molecular entity in which the electronic transition responsible for a given spectral band is approximately localized. The term arose in the dyestuff industry, referring originally to the groupings in the molecule that are responsible for the dye's colour.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1097
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232

chromosome

A self-replicating structure consisting of DNA complexed with various proteins and involved in the storage and transmission of genetic information; the physical structure that contains genes (cf. plasmid). Eukaryotic cells have a characteristic number of chromosomes per cell (cf. ploidy) and contain DNA as linear duplexes. The chromosomes of bacteria consist of double-standed, circular DNA molecules.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 150

chronic toxicity

1. Adverse effects following chronic exposure.

2. Effects which persist over a long period of time whether or not they occur immediately upon exposure or are delayed.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1044

CIDEP (Chemically Induced Dynamic Electron Polarization)

Non-Boltzmann electron spin state population produced in thermal or photochemical reactions, either from a combination of radical pairs (called radical-pair mechanism), or directly from the triplet state (called triplet mechanism), and detected by ESR spectroscopy.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232

CIDNP (Chemically Induced Dynamic Nuclear Polarization)

Non-Boltzmann nuclear spin state distribution produced in thermal or photochemical reactions, usually from colligation and diffusion, or disproportionation of radical pairs, and detected by NMR spectroscopy by enhanced absorption or emission signals.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1097
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232

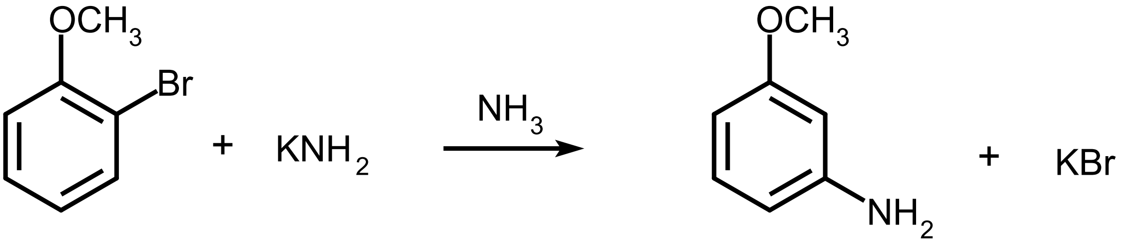
CIEEL (Chemically Initiated Electron Exchange Luminescence)

A type of luminescence resulting from a thermal electron-transfer reaction. Also called catalysed chemiluminescence.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2232

cine-substitution

A substitution reaction (generally aromatic) in which the entering group takes up a position adjacent to that occupied by the leaving group. For example,



See also: tele-substitution

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1097

CIP priority

In the CIP rules the conventional order of ligands established for the purpose of unambiguous designation of stereoisomers. It is deduced by application of sequence rules, the authoritative statement of which appears in R.S. Cahn, C.K. Ingold and V. Prelog, *Angew. Chem. 78*, 413-447 (1966), *Angew. Chem. Internat. Ed. Eng. 5*, 385-415, 511 (1966); and V. Prelog and G. Helmchen, *Angew. Chem. 94*, 614-631 (1982), *Angew. Chem. Internat. Ed. Eng. 21*, 567-583 (1982).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203

circular dichroism (CD)

A spectroscopic method which measures the difference in absorbance of left- and right-handed circularly polarised light by a material, as a function of the wavelength. Most biological molecules, including proteins and nucleic acids, are chiral and show circular dichroism in their ultraviolet absorption bands, which may be used as an indication of secondary structure. Metal centres that are bound to such molecules, even if they have no inherent chirality, usually exhibit CD in absorption bands associated with ligand-based or ligand-metal charge-transfer transitions. CD is frequently used in combination with absorption and *MCD* studies to assign electronic transitions.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1265

cis, *trans*

Descriptors which show the relationship between two ligands attached to separate atoms that are connected by a double bond or are contained in a ring. The two ligands are said to be located *cis* to each other if they lie on the same side of a plane. If they are on opposite sides, their relative position is described as *trans*. The appropriate reference plane of a double bond is perpendicular to that of the relevant σ-bonds and passes through the double bond. For a ring (the ring being in a conformation, real or assumed, without re-entrant angles at the two substituted atoms) it is the mean plane of the ring(s).

For alkenes the terms *cis* and *trans* may be ambiguous and have therefore largely been replaced by the E,Z convention for the nomenclature of organic compounds. If there are more than two entities attached to the ring the use of *cis* and *trans* requires the definition of a reference substituent.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2203
Blue Book (Guide), p. 149

cis conformation

Also contains definition of: *trans* conformation *in polymers*

in polymers

Conformations referring to torsion angles θ (A, B, C, D), where A, B, C, D are main-chain atoms, can be described as: *cis* or synperiplanar (C); gauche or synclinal (G); anticlinal (A); and *trans* or antiperiplanar (T), corresponding to torsion angles within ± 30° of, respectively, 0°, ± 120° and ± 180°. The letters shown in parentheses (upper case C, G, A, T) are the recommended abbreviations. The symbols G^+, G^- (or A^+, G^-, for example) refer to torsion angles of similar type but opposite known sign, i.e. ~ +60°, ~ -60° (or ~ +120°, -120°). The notation G, $\bar{G}$; A, $\bar{A}$ (and T, $\bar{T}$; C, $\bar{C}$ - whenever the torsion angles are not exactly equal to 180° and 0°, respectively) is reserved for the designation of enantiomorph conformations, i.e. conformations of op- posite but unspecified sign. Where necessary, a deviation from the proper value of the torsion angle can be indicated by the sign (~), as in the following examples: G(~); G^+ (~); G^- (~).

Source:
Purple Book, p. 41

cis-

in inorganic nomenclature

A prefix designating two groups occupying adjacent positions in a coordination sphere, not now generally recommended for precise nomenclature purposes.

Source:
Red Book, p. 245

cis-fused

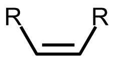
Also contains definition of: *trans*-fused

Steric relations at saturated bridgeheads common to two rings are denoted by cis or trans, followed by a hyphen and placed before the name of the ring system, according to the relative positions of the exocyclic atoms or groups attached to the bridgeheads. Such rings are said to be *cis*-fused or *trans*-fused.

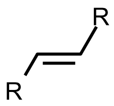
Source:
Blue Book, p. 479

cis-trans isomers

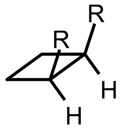
Stereoisomeric olefins or cycloalkanes (or hetero-analogues) which differ in the positions of atoms (or groups) relative to a reference plane: in the *cis*-isomer the atoms are on the same side, in the *trans*-isomer they are on opposite sides.



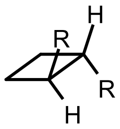
cis



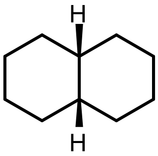
trans



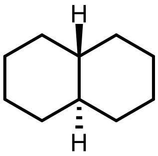
cis



trans



cis



trans

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2204

cisoid conformation [obsolete]

(Usage strongly discouraged).
See: s-cis, s-trans
The terms *cisoid* and *transoid* are also used to describe the stereochemistry of fused ring systems.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2204
Blue Book, p. 478

cistactic polymer

A tactic polymer in which the main-chain double bonds of the configurational base units are entirely in the cis arrangement.

Source:
Purple Book, p. 33

class (a) metal ion

A metal ion that combines preferentially with ligands containing ligating atoms that are the lightest of their Periodic Group.
See also: class (b) metal ion, hard acid

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1097

class (b) metal ion

A metal ion that combines preferentially with ligands containing ligating atoms other than the lightest of their Periodic Group.
See also: class (a) metal ion, hard acid

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1097

class of helix

in polymers

The number of skeletal chain atoms contained within the helix residue.

Source:
Purple Book, p. 79

clathrates

Inclusion compounds in which the guest molecule is in a cage formed by the host molecule or by a lattice of host molecules.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1097

clausius

Non-SI unit of entropy, $\mathrm{Cl} = 4.184\ \mathrm{J\ K^{-1}}$.

Source:
Green Book, 2nd ed., p. 113

clay hybrid

Also contains definitions of: polymer-clay composite, polymer-clay hybrid

Organic–inorganic composite material in which one of the components is a clay, the particles of which are dispersed in a polymer.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1812

clean surface

An experimental surface having no surface contamination observable by means of the used method.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

clean up

in spectrochemical analysis

A process caused by sputtering, trapping (or adsorbing) metallic atoms, gas atoms or molecules on the walls of the vessel or anode. This has the effect of reducing the gas pressure in sealed lamps, and may be useful for cleaning up or gettering unwanted gases.

Source:
Orange Book, p. 149

clearance, $\Delta V / \Delta t$

Also contains definition of: volume rate

Product of the concentration of a component in an output system and the volume flow rate of that output system divided by the concentration of this component in the input system.
Note:
The term mean volume rate is recommended for this quantity.
See also: clearance (in toxicology)

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 966

clearance

in toxicology

1. Volume of blood or plasma or mass of an organ effectively cleared of a substance by elimination (metabolism and excretion) divided by time of elimination.
   Note:
   Total clearance is the sum of the clearances of each eliminating organ or tissue for a given substance.
2. (*in pulmonary toxicology*) Volume or mass of lung cleared divided by time of elimination; used qualitatively to describe removal of any inhaled substance which deposits on the lining surface of the lung.
3. (*in renal toxicology*) Quantification of the removal of a substance by the kidneys by the processes of filtration and secretion; clearance is calculated by relating the rate of renal excretion to the plasma concentration.

See also:clearance, $\Delta V / \Delta t$

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1045

clearing point

The temperature at which the transition between the mesophase with the highest temperature range and the isotropic phase occurs.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 496

CLOGP values

CLOGP values are calculated 1-octanol/water partition coefficients, frequently used in structure-property correlation or quantitative structure-activity relationship (SPC/QSAR) studies.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1140

clone

1. A population of genetically identical cells produced from a common ancestor.
2. Sometimes, 'clone' is also used for a number of recombinant DNA molecules all carrying the same inserted sequence.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 150

closed shell molecular systems

Even-electron atomic or molecular systems whose electron configurations consist of doubly occupied orbitals.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1930

closed system

in spectrochemical analysis

See: mercury flow system *in spectrochemical analysis*

Source:
PAC, 1992, *64*, 261 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XIII. Terms related to chemical vapour generation (IUPAC Recommendations 1992))* on page 263

closo-

An affix used in names to denote a cage or closed structure, especially a boron skeleton that is a polyhedron having all triangular faces.

Source:
Red Book, p. 245
Blue Book, p. 464
PAC, 1972, *30*, 681 *(Nomenclature of Inorganic Boron Compounds)* on page 686

cloud

in atmospheric chemistry

An aerosol of the atmosphere which is dense enough to be perceptible to the eye. Usually refers to an assembly of water droplet aerosols suspended in the atmosphere, although dust clouds are also recognized.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

cluster

A number of metal centres grouped close together which can have direct metal bonding interactions or interactions through a bridging ligand, but are not necessarily held together by these interactions.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1265

cluster analysis

Cluster analysis is the clustering, or grouping, of large data sets (*e.g.*, chemical and/or pharmacological data sets) on the basis of similarity criteria for appropriately scaled variables that represent the data of interest. Similarity criteria (distance based, associative, correlative, probabilistic) among the several clusters facilitate the recognition of patterns and reveal otherwise hidden structures.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1140

cluster ion

in mass spectrometry

An ion formed by the combination of more ions or atoms or molecules of a chemical species often in association with a second species. For example, $[(H_2O)_nH]^+$ is a cluster ion.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

co-ions

1. Ions of low relative molecular mass with a charge of the same sign as that of a given colloidal ion.

   Source:
   PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607
2. In an ion exchanger, mobile ionic species with a charge of the same sign as the fixed ions.

Source:
Orange Book, p. 88

co-oligomer

An oligomer derived from more than one species of monomer.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2300

co-oligomerization

Oligomerization in which a co-oligomer is formed.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2306

co-solvency

in polymers

The dissolution of a polymer in a solvent comprising more than one component, each component of which by itself is a non-solvent for the polymer.

Source:
Purple Book, p. 60

coacervation

Also contains definition of: equilibrium solution

The separation into two liquid phases in colloidal systems. The phase more concentrated in colloid component is the coacervate, and the other phase is the equilibrium solution.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 611

coagulation (flocculation)

in colloid chemistry

When a sol is colloidally unstable (i.e. the rate of aggregation is not negligible) the formation of aggregates is called coagulation or flocculation.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 609
Orange Book, p. 85

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

coal tar pitch

A residue produced by distillation or heat treatment of coal tar. It is a solid at room temperature, consists of a complex mixture of numerous predominantly aromatic hydrocarbons and heterocyclics, and exhibits a broad softening range instead of a defined melting temperature.
Note:
The hydrogen aromaticity in coal tar pitch (ratio of aromatic to total content of hydrogen atoms) varies from 0.7 to 0.9.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 485

coal-derived pitch coke

The primary industrial solid carbonization product obtained from coal tar pitch mainly produced in chamber or delayed coking processes.
Note:
Coal-derived pitch coke, although it exhibits a pregraphitic microstructure, has often a lower graphitizability than petroleum coke. Fractions of coal tar pitches (obtained by extraction or filtration) may form cokes with needle-like structures and have an improved graphitizability. The usually lower graphitizability compared to petroleum coke is due to an inhibition of mesophase growth because of chemical and physical differences of the cokes.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 485

coalescence

in colloid chemistry

The disappearance of the boundary between two particles (usually droplets or bubbles) in contact, or between one of these and a bulk phase followed by changes of shape leading to a reduction of the total surface area. The flocculation of an emulsion, viz. the formation of aggregates, may be followed by coalescence.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

coalification

A geological process of formation of materials with increasing content of the element carbon from organic materials that occurs in a first, biological stage into peats, followed by a gradual transformation into coal by action of moderate temperature (about $500\ \mathrm{K}$) and high pressure in a geochemical stage.
Note:
Coalification is a dehydrogenation process with a reaction rate slower by many orders of magnitude than that of carbonization. Some specific reactions approach completion before others have started. The dehydrogenation remains incomplete. The degree of coalification reached by an organic material in the process of coalification increases progressively and can be defined by means of the measured C/H ratio and of the residual contents of oxygen, sulfur and nitrogen.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 485

codon

The sequence of three consecutive nucleotides that occurs in mRNA which directs the incorporation of a specific amino acid into a protein and includes also the starting or termination signals of protein synthesis.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 150

coefficient

Proportionality constant between two quantities of different dimension.

Source:
ISO 31-0: 1992 *(Quantities and Units - Part 0: General Principles, Units and Symbols.)*

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 966

coefficient of haze (COH)

in atmospheric chemistry

One technique of measurement of the amount of filterable particulate matter suspended in air which has been used in the past depends upon drawing a measured sample of air (usually 1 000 linear feet) through a paper or membrane filter. A measurement is made of the intensity of light transmitted through the dust spot formed relative to that transmitted through an identical clean filter. The dirtiness of the air is reported in terms of the COH unit. This relates to the quantity of particulate material which produces an optical density,

$$\log_{10}\left(\frac{I_0}{I}\right)$$

of 0.01 when measured by light transmission at 400 nm and relative to the transmission of an identical dust-free filter taken as 100%. Thus a filter which transmitted 50% relative to the clean filter has an absorbance of 0.301 or 30.1 COH units. This is not a recommended measure of filterable particulate matter since the size, colour and other properties of the aerosol and the air in which it is suspended affect the results.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

coenzyme

The dissociable, low-relative-molecular-mass active group of an enzyme which transfers chemical groups, hydrogen or electrons. A coenzyme binds with its associated protein (apoenzyme) to form the active enzyme (holoenzyme).

Source:
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

See also:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 150

coextraction

Formation of mixed-species aggregates in a low-polarity organic phase.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2377

cofactors

Organic molecules (cf. coenzymes) or ions (usually metal ions) that are required by an enzyme of its activity. They may be attached either loosely or tightly prosthetic group) to the enzyme. A cofactor binds with its associated protein (apoenzymes), which is functionally inactive, to form the active enzyme (holoenzyme).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 150

coherence length, ζ

Also contains definitions of: electric coherence length*in thin films*, ξ_E, magnetic coherence length*in thin films*, ξ_M

in thin films

The distance over which order is maintained. As an example, there can be long-range atomic or molecular order, i.e. coherence. Coherence lengths are significantly larger than molecular size. Normally, coherence length is estimated from electron, neutron or X-ray scattering and scales the size of ordered domains in material where long range ordering occurs (as in liquid crystals, for example). The term coherence length is also used for the scale characterizing the profile of molecular axis orientation in the distorted, so-called, transition layers formed at a solid/liquid-crystal boundary when an appropriate external field is applied (e.g. when the orientation of anchored surface molecules of a nematic liquid crystal is unaffected by an external field -- magnetic or electric -- whereas the bulk molecules reorient freely). This scale is referred to as electric coherence length, ζ_E or magnetic coherence length, ζ_M, depending on the nature of the applied field.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1675

coherent (derived) unit

of measurement

Derived unit of measurement that may be expressed as a product of powers of base units with the proportionality factor one.

Source:
VIM
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 966

coherent radiation

Radiation emitted by a source when all the elementary waves emitted have a phase difference constant in space and time.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2233

coherent scattering

Also contains definition of: incoherent scattering

Scattering is coherent whenever the phases of the signals arising from different scattering centres are correlated and incoherent whenever these phases are uncorrelated.

Source:
PAC, 1983, *55*, 931 *(Definitions, terminology and symbols in colloid and surface chemistry. Part 1.14: Light scattering (Provisional))* on page 932

coherent source

Also contains definition of: non-coherent source *in spectrochemistry*

in spectrochemistry

Those sources where the radiation has a constant phase relationship between waves spatially as well as temporally, e.g. lasers. Non-coherent optical sources emit radiation which is randomly distributed in phase, spatially as well as temporally. Most sources which are used in spectroscopy and for spectrochemical analysis conform to this latter group.

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1456

coherent structure

Also contains definition of: incoherent structure

If the net of an ordered adsorbed phase is in registry with the lattice of the adsorbent the structure is called coherent, if not it is called incoherent.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

coherent system of units

of measurement

System of units of measurement in which all of the derived units are coherent.
See: coherent (derived) unit *of measurement*, derived unit *of measurement*

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 966

coincidence circuit

An electronic circuit which produces a usable output pulse only when each of its inputs receives a pulse within a specified time interval.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

coincidence resolving time

The greatest time interval that can elapse between the occurrence of two or more consecutive signal pulses, in order that the measuring device processes them as a coincidence.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

coke

A solid high in content of the element carbon and structurally in the non-graphitic state. It is produced by pyrolysis of organic material which has passed, at least in part, through a liquid or liquid-crystalline state during the carbonization process. Coke can contain mineral matter.
Note:
As some parts, at least, of the carbonization product have passed through a liquid or liquid-crystalline state, the resulting non-graphitic carbon is of the graphitizable variety. From a structural viewpoint, the term coke characterizes the state of graphitizable carbon before the beginning of graphitization.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 485

coke breeze

A by-product of coke manufacture; it is the residue from the screening of heat-treated coke. The particle size is less than $10\ \mathrm{mm}$. Generally, coke breeze has a volatile matter content of $<3\ \mathrm{wt.\%}$.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 486

coking

Many reactions involving hydrocarbons and particularly those run at higher temperatures lead to the deposition on the catalyst of high molecular weight compounds of carbon and hydrogen which deactivate the catalyst. This phenomenon is called coking or fouling. Catalysts so deactivated can often be regenerated.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 84

col (saddle point)

A mountain-pass in a potential-energy surface is known as a col or saddle point. It is a point at which the gradient is zero along all coordinates, and the curvature is positive along all but one coordinate, which is the reaction coordinate, along which the curvature is negative.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 158

cold neutrons

Neutrons with a neutron temperature considerably lower than normal room temperature.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

collection

The planned removal from solution of a micro- or macro-component by the intentional formation of a contaminated host precipitate, or by the adsorption or entrapment of the component by an added solid.

Source:
Orange Book, p. 84

collection efficiency

in atmospheric chemistry

A term which characterizes an entire sampling and sample pretreatment procedure, usually represented as a percentage of the original amount of the analyte which is left for measurement (signal formation) after having passed through this procedure. This term also applies to the efficiency of collection of an air pollutant by an arrestment plant. For particulates, the collection efficiency is size related.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2181

collection gas flow system

in spectrochemical analysis

A system in which the analyte is carried to a collecting device called the collector which may be an amalgamator for mercury, a cold trap for some of the more stable hydrides, an absorbing solution in which the analyte is absorbed by some chemical reaction, an electrothermal atomizer or a reservoir.

Source:
PAC, 1992, *64*, 261 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XIII. Terms related to chemical vapour generation (IUPAC Recommendations 1992))* on page 263

collector

in atmospheric chemistry

A device for removing and retaining contaminants from air or other gases; a term which is often applied to cleaning devices in exhaust systems. Also used to designate a device for removing and retaining samples from media in different environmental compartments to be investigated. A collector is sometimes used to describe a scavenger.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2181

collector (scavenger)

A solid substance added to or formed within a solution to collect a micro- or macro-component.

Source:
Orange Book, p. 84

colligation

The formation of a covalent bond by the combination or recombination of two radicals (the reverse of unimolecular homolysis). For example:

$$H_3C^\bullet \quad + \quad {}^\bullet OH \longrightarrow CH_3OH$$

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1097

collimation

The limiting of a beam of radiation to the required dimensions and angular spread.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

collimator

An arrangement of absorbers used for collimation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

collinear reaction

This is a reaction assumed to occur via an activated complex in which all of the atoms directly involved in the process lie along a straight line.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 158

collision complex

An ensemble formed by two reaction partners for which the distance is the sum of their van der Waals radii. As such it constitutes a subclass of the species indicated as encounter complex.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2233

collision cross-section, σ

In simple hard sphere collision theory the area of the circle with radius equal to the collision diameter.

Source:
Green Book, 2nd ed., p. 56

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 158

collision density, Z_{AA}

Total collision frequency for all molecules within a volume divided by that volume.

Source:
Green Book, 2nd ed., p. 56

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 158

collision diameter, d

In simple hard sphere collision theory the sum of radii of two colliding spherical particles.
See also: collision cross-section

Source:
Green Book, 2nd ed., p. 56

collision efficiency, B_c

Synonym: de-energization efficiency

The collision efficiency, or de-energization efficiency, is defined by:

$$k_{-1} = B_c \, k_{-1}^{sc}$$

where k_{-1} is the rate constant for a particular substance M when it brings about the de-energization process

$$\mathrm{M} + \mathrm{A^*} \longrightarrow \mathrm{M} + \mathrm{A}$$

and k_{-1}^{sc} is the corresponding rate constant for a reference molecule $\mathrm{M_r}$ that de-energizes $\mathrm{A^*}$ on every collision; that is, the reference molecule $\mathrm{M_r}$ undergoes strong collisions, and by definition has a collision efficiency B_c of unity. The species $\mathrm{A^*}$ is usually in a vibrationally-excited state, and A has energy less than that required for reaction to occur.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 159

collision frequency, $z_{\mathrm{A}}(\mathrm{A})$

Average number of collisions experienced by a molecule **A** with other molecules **A** (or **B**) in a time interval divided by that time interval.

Source:
Green Book, 2nd ed., p. 56

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 159

collision number

Now called collision density.

Source:
Green Book, 2nd ed., p. 56
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 160

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2181

collision theory

Various collision theories, dealing with the frequency of collision between reactant molecules, have been put forward. In the earliest theories reactant molecules were regarded as hard spheres, and a collision was considered to occur when the distance d between the centres of two molecules was equal to the sum of their radii. For a gas containing only one type of molecule, **A**, the collision density is given by simple collision theory as:

$$Z_{\mathrm{AA}} = \frac{\sqrt{2}\,\pi\,\sigma^2\,u\,N_{\mathrm{A}}^{\;2}}{2}$$

Here N_{A} is the number density of molecules and u is the mean molecular speed, given by kinetic theory to be $\sqrt{\frac{8\,k_{\mathrm{B}}\,T}{\pi\,m}}$, where m is the molecular mass, and $\sigma = \pi\,d_{\mathrm{AA}}^{\;2}$. Thus:

$$Z_{\mathrm{AA}} = 2\,N_{\mathrm{A}}^{\;2}\,\sigma^2\sqrt{\frac{\pi\,k_{\mathrm{B}}\,T}{m}}$$

The corresponding expression for the collision density Z_{AB} for two unlike molecules **A** and **B**, of masses m_{A} and m_{B} is:

$$Z_{\mathrm{AB}} = N_{\mathrm{A}}\,N_{\mathrm{B}}\,\sigma^2\sqrt{\frac{\pi\,k_{\mathrm{B}}\,T}{\mu}}$$

where μ is the reduced mass $\frac{m_{\mathrm{A}}\,m_{\mathrm{B}}}{m_{\mathrm{A}} + m_{\mathrm{B}}}$, and $\sigma = \pi\,d_{\mathrm{AB}}^{\;2}$. For the collision frequency factor these formulations lead to the following expression:

$$z_{\mathrm{AA}} \ \text{or}\ z_{\mathrm{AB}} = L\,\sigma^2\sqrt{\frac{8\,\pi\,k_{\mathrm{B}}\,T}{\mu}}$$

where L is the Avogadro constant. More advanced collision theories, not involving the assumption that molecules behave as hard spheres, are known as generalized kinetic theories.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 160

collision-induced dissociation

in mass spectrometry

An ion/neutral species process wherein the projectile ion is dissociated as a result of interaction with a target neutral species. This is brought about by conversion of part of the translational energy of the ion to internal energy in the ion during the collision.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

collisional activation (collisionally activated dissociation)

in mass spectrometry

An ion/neutral species process wherein excitation of a projectile ion of high translational energy is brought about by the same mechanism as in collision-induced dissociation. (The ion may decompose subsequently.)

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1554

collisional broadening

Also contains definitions of: foreign-gas broadening, resonance broadening
of a spectral line

, van der Waals broadening
of a spectral line

of a spectral line

Collisions of the emitting or absorbing particle with other particles cause collisional broadening as well as collisional shift of the spectral line. When collisions occur between unlike, neutral particles the term foreign-gas broadening is used, or van der Waals' broadening when both collision partners are neutral. When the colliding particles are of the same species, the term resonance broadening is employed. The term Lorentz broadening was previously used for neutral particle collision broadening, and Holtsmark broadening for cases of van der Waals' broadening when collisions took place with like particles. Both terms are now discouraged. Stark broadening refers to collisions with charged particles or particles with a strong permanent electrical dipole moment. Whereas a strong chaotic electrical field causes Stark broadening, an applied static electrical field induces a Stark shift.

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1463
Orange Book, p. 122

collisional excitation

in mass spectrometry

An ion/neutral species process wherein there is an increase in the reactant ion's internal energy at the expense of the translational energy of either (or both) of the reacting species. The scattering angle may be large.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

colloid

A short synonym for colloidal system.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 605

colloid osmotic pressure (Donnan pressure)

The pressure difference which has to be established between a colloidal system and its equilibrium liquid to prevent material transfer between the two phases when they are separated by a membrane, permeable to all components of the system, except the colloidal ones.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 615

colloidal

The term refers to a state of subdivision, implying that the molecules or polymolecular particles dispersed in a medium have at least in one direction a dimension roughly between $1\ \mathrm{nm}$ and $1\ \mu\mathrm{m}$, or that in a system discontinuities are found at distances of that order.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 605

colloidal carbon

A particulate carbon with particle sizes below *ca.* $1000\ \mathrm{nm}$ in at least one dimension.
Note:
Colloidal carbon exists in several morphologically distinct forms.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 486

colloidal dispersion

A system in which particles of colloidal size of any nature (e.g. solid, liquid or gas) are dispersed in a continuous phase of a different composition (or state). The name dispersed phase for the particles should be used only if they have essentially the properties of a bulk phase of the same composition.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 605

colloidal electrolyte

An electrolyte which gives ions of which at least one is of colloidal size. This term therefore includes hydrophobic sols, ionic association colloids, and polyelectrolytes.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

colloidal gel

Gel in which the network component comprises particles of colloidal dimensions.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1807

colloidal network

Network comprising particles of colloidal dimensions.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1813

colloidal processing

Sol-gel processing in which a network of precipitated colloidal particles is treated by a conventional processing technique, such as cold pressing, hot pressing or sintering, in order to produce a ceramic article.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1821

colloidal suspension

A suspension in which the size of the particles lies in the colloidal range.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 606

colloidally stable

Particles which do not aggregate at a significant rate: the precise connotation depends on the type of aggregation under consideration. For example, a concentrated paint is called stable by some people because oil and pigment do not separate out at a measurable rate, and unstable by others because the pigment particles aggregate into a continuous network.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 609

color scale

Series of ordered numbers that represents observable gradations of a given attribute or gradations of a combination of attributes of color perception.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 315

colorimeter

An instrument used for colour measurement based on optical comparison with standard colours.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2181

colour indicator

Also contains definitions of: one-colour indicator, two-colour indicator

An indicator which is classified as one- or two-colour, depending on whether it is colourless on one side of the transition interval or possesses a different colour on each side of this range.

Source:
Orange Book, p. 48

colourability

Ability of a colourless or slightly coloured photochromic material to develop colour.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 315

column chromatography

A separation technique in which the stationary bed is within a tube. The particles of the solid stationary phase or support coated with a liquid stationary phase may fill the whole inside volume of the tube (packed column) or be concentrated on or along the inside tube wall leaving an open, unrestricted path for the mobile phase in the middle part of the tube (open-tubular column).

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 825

column

in chromatography

The tube and the stationary phase contained within, through which the mobile phase passes.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831
Orange Book, p. 97

column volume, V_c

in chromatography

The geometric volume of the part of the tube that contains the packing:

$$V_c = A_c L$$

where A_c is the internal cross-sectional area of the tube and L the length of the packed part of the column. In the case of wall-coated open-tubular columns the column volume corresponds to the geometric volume of the whole tube having a liquid or a solid stationary phase on its wall.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 832

See also:
Orange Book, p. 100

comb macromolecule

Also contains definitions of: brush macromolecule, regular comb macromolecule

A macromolecule comprising a main chain with multiple trifunctional branch points from each of which a linear side-chain emanates.
Notes:

1. If the subchains between the branch points of the main chain and the terminal subchains of the main chain are identical with respect to constitution and degree of polymerization, and the side chains are identical with respect to constitution and degree of polymerization the macromolecule is termed a regular comb macromolecule.
2. If at least some of the branch points are of functionality greater than three, the macromolecule may be termed a brush macromolecule.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2296

comb polymer

A polymer composed of comb macromolecules.
See also: regular polymer

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2304

combination electrode

An ion-selective electrode and an external reference electrode combined in a single unit, thereby avoiding the need for a separate external reference electrode.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2528

combined sample

A sample obtained by removing specific fractions by separation or selection techniques (e.g. heavy liquid, magnetic, sieving, etc.), analysing the fractions separately, and combining the results mathematically. When not combined, the sample is a modified sample. This term should not be confused with composite sample.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1204

combustion gas

A gas or vapour produced in furnaces, combustion chambers or in open burning.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2181

commensurate–incommensurate transition

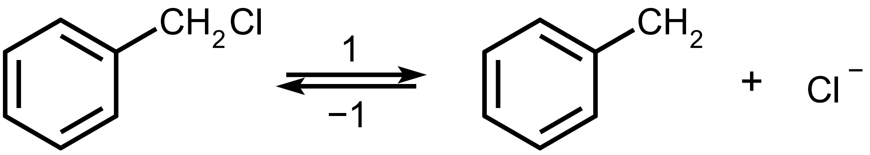
Also contains definition of: lock-in state

A transition between two states having magnetic or crystallographic structures with a basic lattice and an imposed super-periodicity. In the commensurate (lock-in) state this super-periodicity is a simple rational multiple of the basic unit cell. In the incommensurate state the ratio of the super-periodicity repeat distance to the basic lattice repeat distance is irrational and may show continuous variation with variation in some degree of freedom (e.g. temperature, pressure, composition) of the system. Example: The transition of Rb_2ZnCl_4 from an incommensurate structure to a commensurate structure at the lock-in temperature, T_L, which is dependent on the crystal growth method and varies in the range 128 K to 190 K.
Note:
A commensurate–incommensurate transition also occurs in liquid-crystal systems where there is an incommensurability in the packing of dimers in relation to monomers.

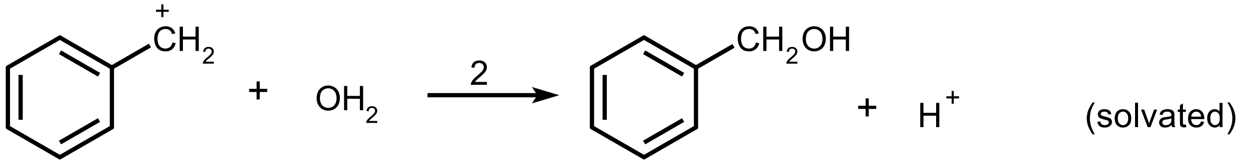
Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 579

common-ion effect (on rates)

A reduction in the rate of certain reactions of a substrate RX in solution [by a path that involves a pre-equilibrium with formation of R^+ (or R^-) ions as reaction intermediates] caused by the addition to the reaction mixture of an electrolyte solute containing the 'common ion' X^- (or X^+). For example, the rate of solvolysis of diphenylmethyl chloride in acetone- water is reduced by the addition of salts of the common ion Cl^- which causes a decrease in the quasi-equilibrium concentration of the diphenylmethyl cation in the scheme:



(free ions,*not*ion pairs)



This phenomenon is a direct consequence of the mass-law effect on ionization equilibria in electrolytic solution. More generally, the common-ion effect is the influence of the 'common ion' on the reactivity due to the shift of the dissociation equilibrium. It may also lead to an enhancement of the rate of reaction.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1098

communities (consortia, syntrophic or synergistic associations)

Naturally occuring groups of different (micro)organisms inhabiting a common environment, interacting with each other, especially through food relationships and relatively independent of other groups. Communities may be of varying sizes, and larger communities may contain smaller ones.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 150

comparative molecular field analysis (CoMFA)

Comparative Molecular Field Analysis (CoMFA) is a 3D-QSAR method that uses statistical correlation techniques for the analysis of the quantitative relationship between the biological activity of a set of compounds with a special alignment, and their three-dimensional electronic and steric properties. Other properties, such as hydrophobicity and H-bonding, can also be incorporated into the analysis.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1140

comparator

in radioanalytical chemistry

A known amount of element that is simultaneously irradiated with the test portion in the context of activation analysis. If one comparator is used (single comparator method), it is essentially identical to a flux monitor (expect that this term is not necessarily linked to activation analysis).

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

compartmental analysis

Mathematical process leading to a model of transport of a substance in terms of compartments and rate constants, usually taking the form

$$C = A\,\mathrm{e}^{-\alpha\,t} + B\,\mathrm{e}^{-\beta\,t} \ldots$$

where each exponential term represents one experiment. C is the substance concentration; A, B,... are proportionality constants; α, β,... are rate constants; and t is time.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1045

compatible polymer blend

Immiscible polymer blend that exhibits macroscopically uniform physical properties.
Note:
The macroscopically uniform properties are usually caused by sufficiently strong interactions between the component polymers.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1817

compensation effect

In a considerable number of cases plots of $T\,\Delta^{\ddagger}S$ vs. $\Delta^{\ddagger}H$, for a series of reactions, e.g. for a reaction in a range of different solvents, are straight lines of approximately unit slope. Therefore, the terms $\Delta^{\ddagger}H$ and $T\,\Delta^{\ddagger}S$ in the expression partially compensate, and

$$\Delta^{\ddagger}G = \Delta^{\ddagger}H - T\,\Delta^{\ddagger}S$$

often is a much simpler function of solvent (or other) variation than $\Delta^{\ddagger}H$ or $T\,\Delta^{\ddagger}S$ separately.
See also: isokinetic relationship

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1098

compensation
in catalysis

For the process:

$$k = A\,\mathrm{e}^{\frac{-E}{R\,T}}$$

where k is a rate constant, A the frequency factor and E the activation energy, A and E sometimes exhibit compensation, i.e. they change in the same direction with change in catalyst for a given reaction or with change in reaction for a given catalyst.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 82

compensation

in stereochemistry

1. For internal compensation, see compound.
2. ***See:*** external compensation

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2204

competition

See: composite mechanism

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 160

competitive binding assay

An assay based on the competition between a labelled and an unlabelled ligand in the reaction with a receptor binding agent (e.g. antibody, receptor, transport protein).

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

competitive inhibition

of catalysis

The reduction in rate due to reduction or loss of activity of a catalyst caused by adsorption of poison which is not greatly preferred to adsorption of reactant.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 83

complementary binding sites

See: binding site

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1098

complementary DNA (cDNA)

A single-stranded DNA molecule with a nucleotide sequence that is complementary to an RNA molecule; cDNA is formed by the action of the enzyme reverse transcriptase on an RNA template. After conversion to the double-stranded form, cDNA is used for molecular cloning or for hybridization studies.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 150

complete active space self-consistent field (CASSCF)

Computational scheme employed in multiconfigurational SCF theory especially suitable for studies of reactivity of excited states. The wavefunction is defined by selecting the set of active orbitals involved in the excitation or chemical reaction under investigation and is constructed as a linear expansion in the set of configuration functions that can be generated by occupying the active orbitals in all ways consistent with an overall spin and space symmetry (full configuration interaction, CI).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 315

complete active space self-consistent field second-order perturbation theory (CASPT2)

Theoretical scheme suitable for computations of accurate excitation energies and reaction barriers. In the first step, electron correlation is taken into account only to a certain extent by using a *CASSCF* formalism (the so called non-dynamic correlation), whereas the remaining electron correlation (the so called dynamic correlation) is included through the use of second-order perturbation theory.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 316

complex

A molecular entity formed by loose association involving two or more component molecular entities (ionic or uncharged), or the corresponding chemical species. The bonding between the components is normally weaker than in a covalent bond. The term has also been used with a variety of shades

of meaning in different contexts: it is therefore best avoided when a more explicit alternative is applicable. In inorganic chemistry the term 'coordination entity' is recommended instead of 'complex'.
See also: activated complex, adduct, charge transfer complex, electron-donor-acceptor complex, encounter complex, inclusion complex, σ-adduct, π-adduct, transition state

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1098

complex coacervation

Coacervation caused by the interaction of two oppositely charged colloids.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 611

complex mechanism

This term is sometimes applied to an elementary reaction which proceeds via an intermediate species having a lifetime longer than a few rotational periods, in contrast to a direct reaction. However, in view of the danger of confusion with a reaction occurring in more than one step (a composite reaction) this usage is not to be recommended; it is better to use the terms complex-mode mechanism or complex-mode reaction.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 160

complex reaction

See: composite mechanism

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 161

complex-mode reaction

An elementary reaction which proceeds via an intermediate species having a lifetime longer than a few rotational periods is known as a complex-mode reaction, or as an indirect reaction.
See also: direct reaction

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 160

component

Constituent of a mixture the amount or concentration of which can be varied independently. The number of components in a given system is the minimum number of independent species necessary to define the composition in all the phases of a system. It may vary with external conditions since additional chemical equilibria reduce the number of components. The term component is also often used in the more general sense as defined here under constituent.

Source:
Physical Chemistry Division, unpublished

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 966

composite

Multicomponent material comprising multiple, different (non-gaseous) phase domains in which at least one type of phase domain is a continuous phase.
Note:
A foamed substance, which is a multiphase material that consists of a gas dispersed in a liquid or solid, is not normally considered to be a composite.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1810

composite mechanism

Also contains definition of: negative feedback

A reaction that involves more than one elementary reaction is said to occur by a composite mechanism. The terms complex mechanism, indirect mechanism, and step-wise mechanism are also commonly used. There are two main kinds of evidence for a composite mechanism:

1. The kinetic equation for the reaction does not correspond to its stoichiometry.
2. There is experimental evidence, direct or indirect, for intermediates of such a nature that it is necessary to conclude that more than one elementary reaction is involved.

There are many types of composite mechanisms, for example:

1. Reactions occurring in parallel, such as:

$$\mathrm{A} \longrightarrow \mathrm{Y}$$

$$\mathrm{A} \longrightarrow \mathrm{Z}$$

are called parallel reactions or simultaneous reactions. When there are simultaneous reactions there is sometimes competition, as in the scheme:

$$A + B \longrightarrow Y$$

$$A + C \longrightarrow Z$$

where B and C compete with one another for A.

2. Reactions occurring in forward and reverse directions are called opposing reactions:

$$A + B \rightleftharpoons Z$$

3. Reactions occurring in sequence, such as

$$A \longrightarrow X \longrightarrow Y \longrightarrow Z$$

are known as consecutive reactions.

4. Reactions are said to exhibit feedback if a substance formed in one step affects the rate of a previous step. For example, in the scheme:

$$A \longrightarrow X \longrightarrow Y \longrightarrow Z$$

The intermediate Y may catalyse the reaction $A \longrightarrow X$ (positive feedback) or it may inhibit it (negative feedback).

5. Chain reactions

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 161

composite membrane

Membrane having chemically or structurally distinct layers.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1481

composite reaction

A chemical reaction for which the expression for the rate of disappearance of a reactant (or rate of appearance of a product) involves rate constants of more than a single elementary reaction. Examples are 'opposing reactions' (where rate constants of two opposed chemical reactions are involved), 'parallel reactions' (for which the rate of disappearance of any reactant is governed by the rate constants relating to several simultaneous reactions to form different respective products from a single set of reactants), and stepwise reactions.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1098
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2293

composite sample

Often prepared as a representative mixture of several different (usually bulk) samples, and from which the laboratory sample is taken.

Source:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1465

composition of pure air

in atmospheric chemistry

The composition of air is variable with respect to several of its components (e.g. CH_4, CO_2, H_2O) so 'pure' air has no precise meaning; it is commonly considered to be air which is free of dust, aerosols and reactive gaseous contaminants of anthropogenic origin. The composition of the major components in dry air is relatively constant (percent by volume given): nitrogen, 78.084; oxygen, 20.946; argon, 0.934; carbon dioxide, 0.033; neon, 0.0018; helium, 0.000524; methane, 0.00016; krypton, 0.000114; hydrogen 0.00005; nitrous oxide, 0.00003; xenon, 0.0000087. The concentrations of carbon dioxide, methane, nitrous oxide, the chlorofluorocarbons and some other species of anthropogenic origin are increasing measurably with time. Relative clean air which is free of most reactive anthropogenic pollution (NO, NO_2, SO_2, non-methane hydrocarbons, etc.), often used as a reference sample in the calibration and operation of instruments, is purchased under the designation of zero air.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

compositional heterogeneity

of polymers

The variation in elemental composition from molecule to molecule usually found in copolymers.

Source:
Purple Book, p. 52

compressibility factor

See: compression factor

Source:
Green Book, 2nd ed., p. 49

compression factor, *Z*

Product of pressure and molar volume divided by the gas constant and thermodynamic temperature. For an ideal gas it is equal to 1.

Source:
Green Book, 2nd ed., p. 49

comproportionation

The reverse of disproportionation. The term 'symproportionation' is also used.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1098

Compton effect

Synonym: Compton scattering

The elastic scattering of a photon by an electron which afterwards occurs as a free electron. Part of the energy and momentum of the incident photon is transferred to the electron and the remaining part is carried away by the scattered photon. Synonymous with Compton scattering

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

Compton electron

The energetic electron resulting from the Compton effect.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

computational chemistry

Computational chemistry is a discipline using mathematical methods for the calculation of molecular properties or for the simulation of molecular behaviour. It also includes, *e.g.*, synthesis planning, database searching, combinatorial library manipulation.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1141

computational photochemistry

Aspects of research that address the study of photochemical events by means of computer simulations using specialized software tools and strategies in order to get an understanding of the process at a microscopic level. The aim is to uncover the mechanism of known photochemical processes, design new photochemical systems, and predict molecular properties that are experimentally inaccessible.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 316

computer-assisted drug design (CADD)

Computer-assisted drug design involves all computer-assisted techniques used to discover, design and optimize biologically active compounds with a putative use as drugs.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1141

computer-assisted molecular design (CAMD)

Computer-assisted molecular design involves all computer-assisted techniques used to discover, design and optimize compounds with desired structure and properties.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1141

computer-assisted molecular modeling (CAMM)

Computer-assisted molecular modeling is the investigation of molecular structures and properties using computational chemistry and graphical visualization techniques.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1141

concave isotherm

in chromatography

Distribution isotherm, the slope of which is continuously increasing.
Note:
The resulting chromatographic peak is fronting. In gas-liquid chromatography, overloading often results in a concave isotherm.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1593

concentration

1. Group of four quantities characterizing the composition of a mixture with respect to the volume of the mixture (mass, amount, volume and number concentration).
2. Short form for amount (of substance) concentration (substance concentration in clinical chemistry).

Source:
Green Book, 2nd ed., p. 42
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 966

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2181

concentration depolarization

Loss of emission anisotropy due to transfer of electronic excitation from photo-selected molecules to other molecules with different orientations.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 316

concentration distribution ratio, D_c

in chromatography

The ratio of the analytical concentration of a component in the stationary phase to its analytical concentration in the mobile phase.

$$D_{\mathrm{c}} = \frac{\text{amount of component} \Big/ \text{cm}^3 \text{of stationary phase}}{\text{amount of component} \Big/ \text{cm}^3 \text{of mobile phase}}$$

Source:
Orange Book, p. 106

concentration factor **[obsolete]**

in solvent extraction

Use of this term is not recommended.
See: extraction factor

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2381

concentration gradient, grad C

Differential change in concentration of a component in a given direction in a small distance divided by the distance in that direction.
Notes:

1. It is a vector quantity.
2. May be expressed as amount-of-substance, mass, number, volume, concentration gradient.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 967

concentration in experimental surface (or surface concentration)

The amount of the material of interest divided by the total amount of substances in the volume of interest. Concentration may be defined in terms of numbers of atoms (particles) (ppma) or in terms of weight ($\frac{\mu g}{g}$).

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2246

concentration overpotential

The concentration overpotential of an electrode reaction at a given electrode current density (c.d.) is basically the difference in equilibrium potentials across the diffusion layer. More precisely, it is the potential of a reference electrode (of the same electrode reaction as the working electrode) with the interfacial concentrations which establish themselves at c.d., relative to the potential of a similar reference electrode with the concentrations of the bulk solution. From such a measured potential difference, with c.d. flowing, one needs to subtract the ohmic potential drop prevailing between the two electrodes.

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1838

concentration thermometric technique **[obsolete]**

in enthalpimetric analysis

See: direct injection enthalpimetry

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2490

concentration-cell corrosion

The local variation of the corrosion rate due to the action of a corrosion cell resulting from inhomogeneous composition of the environment.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 22

concentration-sensitive detector

in chromatography

A device the response of which is proportional to the concentration of a sample component in the eluent.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 849

concerted process

Two or more primitive changes are said to be concerted (or to constitute a concerted process) if they occur within the same elementary reaction. Such changes will normally (though perhaps not inevitably) be 'energetically coupled'. (In the present context the term 'energetically coupled' means that the simultaneous progress of the primitive changes involves a transition state of lower energy than that for their successive occurrence.) In a concerted process the primitive changes may be synchronous or asynchronous.
See also: bifunctional catalysis, potential-energy (reaction) surface

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1098

concerted reaction

A single-step reaction through which reactants are directly transformed into products, *i.e.*, without involvement of any intermediates.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1930

condensation

in atmospheric chemistry

The physical process of converting a material from a gaseous or vapour phase to a liquid or solid phase; this commonly results when the temperature is lowered and/or the vapour pressure of the material is increased. The tendency exists for condensation to occur when the partial pressure of a given component of a gaseous mixture at a given temperature exceeds the vapour pressure of the liquid or solid form of that component at the given temperature.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2182

condensation nuclei (CN)

in atmospheric chemistry

Particles, either liquid or solid, or ions upon which condensation of water vapour (or other substances) begins in the atmosphere. Condensation nuclei are usually very small hygroscopic aerosols ($0.001\ \mu m$ to $0.1\ \mu m$ in diameter), but these are not as abundant as the smaller particles. The number of CN which are active (initiate condensation) in a given air mass may be a function of the relative humidity. Usually CN are counted as the active nuclei at about 300% relative humidity, while cloud condensation nuclei (CCN) are counted as the number of active nuclei at relative humidity less than or equal to 102%.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2182

condensation polymerization (polycondensation)

Polymerization by a repeated condensation process (i.e. with elimination of simple molecules).

Source:
Purple Book, p. 18

condensation reaction

A (usually stepwise) reaction in which two or more reactants (or remote reactive sites within the same molecular entity) yield a single main product with accompanying formation of water or of some other small molecule, e.g. ammonia, ethanol, acetic acid, hydrogen sulfide. The mechanism of many condensation reactions has been shown to comprise consecutive addition and elimination reactions, as in the base-catalysed formation of (*E*)-but-2-enal (crotonaldehyde) from acetaldehyde, *via* 3-hydroxybutanal (aldol). The overall reaction in this example is known as the aldol condensation. The term is sometimes also applied to cases where the formation of water or another simple molecule does not occur, as in 'benzoin condensation'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1099

conditional (formal) potential

Conditional (formal) potential, $E^{0'}$,is related to the potential of a cell reaction, E_{cell}, by an equation analogous to that relating E_{cell} to the standard potential E_0, with the activity, a_i, replaced by any composition variable, c_i (to be indicated by a subscript). For example:

$$E_{\text{cell}} = E_{\text{c}}^{0'} - \frac{RT}{nF} \sum_i \nu_i \ln c_i$$

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 505

conditioning

in solvent extraction

Synonymous with pre-equilibration.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2377

conductance, *G*

See: electric conductance

Source:
Green Book, 2nd ed., p. 15
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 970

conducting polymer

Polymeric material that exhibits bulk electric conductivity.
Notes:

1. ***See also:*** conductivity.
2. The electric conductivity of a conjugated polymer is markedly increased by doping it with an electron donor or acceptor, as in the case of polyacetylene doped with iodine.
3. A polymer showing a substantial increase in electric conductivity upon irradiation with ultraviolet or visible light is called a photoconductive polymer; an example is poly(*N*-vinylcarbazole) (***See also:*** photoconductivity).
4. A polymer that shows electric conductivity due to the transport of ionic species is called an ion-conducting polymer; an example is sulfonated polyaniline. When the transported ionic species is a proton as, *e.g.*, in the case of fuel cells, it is called a proton-conducting polymer.
5. A polymer that shows electric semiconductivity is called a semiconducting polymer (***See also:*** semiconductor).
6. Electric conductance of a non-conducting polymer can be achieved by dispersing conducting particles (*e.g.,* metal, carbon black) in the polymer. The resulting materials are referred to as *conducting* polymer composites or solid polymer-electrolyte composites.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 898

conducting polymer composite

Electrically-conducting composite comprising a non-conducting polymer matrix and an electrically-conducting material.
Note:
Examples of the electrically-conducting materials are carbon black and metal particles.
See also: solid polymer electrolyte

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2069

conduction band

A vacant or only partially occupied set of many closely spaced electronic levels resulting from an array of a large number of atoms forming a system in which the electrons can move freely or nearly so. This term is usually used to describe the properties of metals and semiconductors.
See: bandgap energy, Fermi level, valence band

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2233

conductivity, γ, σ

Reciprocal of resistivity. This quantity is a tensor in an anisotropic medium. It was formerly called specific conductance.

Source:
Green Book, 2nd ed., p. 15
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 967

confidence level

The probability of covering the expected value of an estimated parameter with an interval estimated for the parameter (symbol $1-\alpha$). The confidence level can be expressed as a number between 0 and 1, or in percent. The complementary quantity is known as the significance level.
Note:
In some cases the confidence level is dictated by the needs of the situation. In all other instances, use of $1-\alpha=0.95$ is recommended.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 599

confidence limits (about the mean)

Symmetric confidence limits ($\pm C$) about the estimated mean, which cover the population mean with probability $1-\alpha$. The quantity C is calculated by the formula:

$$C = \frac{t_{\mathrm{p},\nu} s}{\sqrt{n}}$$

Here $t_{\mathrm{p},\nu}$, is the critical value from the t- (or Student) distribution function corresponding to the confidence level $1-\alpha$ and degrees of freedom ν. The symbol p represents the percentile (or percentage point) of the t-distribution. For 1-sided intervals, $p = 1-\alpha$; for 2-sided intervals, $p = 1-\frac{\alpha}{2}$. In each case, the confidence level is $1-\alpha$. The confidence interval is given as $\bar{x} \pm C$.
Note:
If the population standard deviation σ is known, confidence limits about a single result may be calculated with the formula:

$$C = t_{\mathrm{p},\infty}\,\sigma$$

The coefficient $t_{\mathrm{p},\infty}$, is the limiting value of the t-distribution function for $\nu = \infty$ at confidence level $1-\alpha$. This is identical to z_{p}, the pth percentage point of the standard normal variate.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 601

configuration (electronic)

A distribution of the electrons of an atom or a molecular entity over a set of one-electron wavefunctions called orbitals, according to the Pauli principle. From one configuration several states with different multiplicities may result. For example, the ground electronic configuration of the oxygen molecule (O_2) is: $1\sigma_{\mathrm{g}}^2$, $1\sigma_{\mathrm{u}}^2$, $2\sigma_{\mathrm{g}}^2$, $2\sigma_{\mathrm{u}}^2$, $1\pi_{\mathrm{u}}^4$, $3\sigma_{\mathrm{g}}^2$, $1\pi_{\mathrm{g}}^2$ resulting in the ${}^3\Sigma_{\mathrm{g}}$, ${}^1\Delta_{\mathrm{g}}$ and ${}^1\Sigma_{\mathrm{g}}^+$ multiplets.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1099
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2233

configuration interaction (CI)

The mixing of many-electron wavefunctions constructed from different electronic configurations to obtain an improved many-electron state.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2233

configuration (stereochemical)

In the context of stereochemistry, the term is restricted to the arrangements of atoms of a molecular entity in space that distinguishes stereoisomers, the isomerism between which is not due to conformation differences.
See also: absolute configuration, relative configuration

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2204
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1099

configurational base unit

in polymers

A constitutional repeating unit in a regular macromolecule, a regular oligomer molecule, regular block or a regular chain, the configuration of which is defined at least at one site of stereoisomerism in the main chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2291

configurational disorder

in polymers

Structural disorder resulting from the statistical co-crystallization of different configurational repeating units.

Source:
Purple Book, p. 80

configurational homosequence

in polymers

A constitutional homosequence in which the relative or absolute configuration is defined at one or more sites of stereoisomerism in each constitutional unit in the main chain of a polymer molecule.

Source:
Purple Book, p. 36

configurational repeating unit

in polymers

The smallest set of successive configurational base units that prescribes configurational repetition at one or more sites of stereoisomerism in the main chain of a regular macromolecule, a regular oligomer molecule, a regular block or a regular chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2291

configurational sequence

in polymers

The whole or part of a chain comprising one or more species of configurational unit(s) in defined sequence.
Note:
Configurational sequences comprising two configurational units are termed diads, those with three such constitutional units triads, and so on. In order of increasing sequence lengths they are called tetrads, pentads, hexads, heptads, octads, nonads, decads, undecads, etc.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2299

configurational unit

in polymers

A constitutional unit having at least one site of defined stereoisomerism.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2291

conformation

The spatial arrangement of the atoms affording distinction between stereoisomers which can be interconverted by rotations about formally single bonds. Some authorities extend the term to include inversion at trigonal pyramidal centres and other polytopal rearrangements.
See also: conformer, bisecting conformation, eclipsing conformation, chair, boat, twist, crown conformation, envelope conformation, half-chair, staggered conformation, tub conformation

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2204
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1099

conformational analysis

The assessment of the relative energies (or thermodynamic stabilities), reactivities, and physical properties of alternative conformations of a molecular entity, usually by the application of qualitative or semi-quantitative rules or by semi-empirical calculations.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2204

conformational analysis

in drug design

Conformational analysis consists of the exploration of energetically favourable spatial arrangements (shapes) of a molecule (conformations) using molecular mechanics, molecular dynamics, quantum chemical calculations or analysis of experimentally-determined structural data, *e.g.*, NMR or crystal structures.
Molecular mechanics and quantum chemical methods are employed to compute conformational energies, whereas systematic and random searches, Monte Carlo, molecular dynamics, and distance geometry are methods (often combined with energy minimization procedures) used to explore the conformational space.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1141

conformational disorder

in polymers

Structural disorder resulting from the statistical coexistence within the crystals of identical configurational units with different conformations.

Source:
Purple Book, p. 80

conformer

One of a set of stereoisomers, each of which is characterized by a conformation corresponding to a distinct potential energy minimum.
See also: rotamer

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2204

congener

One of two or more substances related to each other by origin, structure, or function.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1046

conglomerate

See: racemic conglomerate

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2204

congruent transition

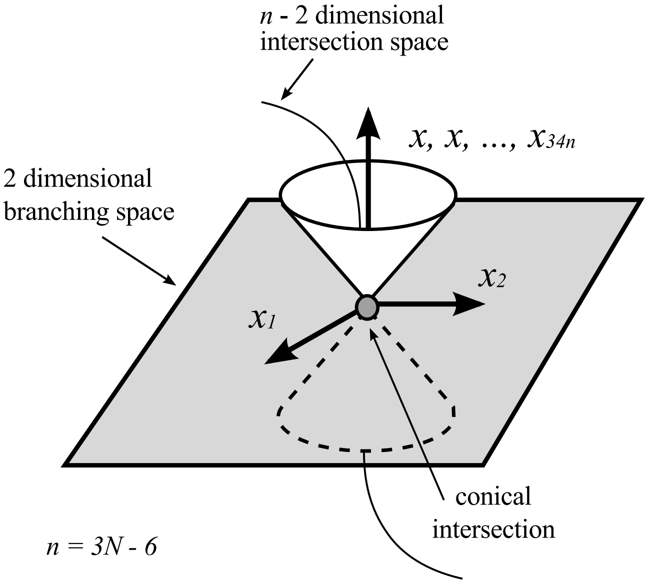
A transition in which the two-phase equilibrium of melting, vaporization or allotropism of a compound involves phases of the same composition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 579

conical intersection

Point of crossing between two electronic states of the same spin multiplicity (most commonly singlets or triplets).
Notes:

1. In a polyatomic molecule two potential energy surfaces are allowed to cross along a $(3N - 8)$-dimensional subspace of the $(3N - 6)$-dimensional nuclear coordinate space (the intersection space) even if they have the same spatial/spin symmetry (N is the number of nuclei). Each point of the intersection space corresponds to a conical intersection. If the energy is plotted against two special internal geometrical coordinates, $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, which define the so-called branching plane, the potential energy surface would have the form of a double cone in the region surrounding the degeneracy. In the remaining $(3N - 8)$ directions, the energies of the ground and excited state remain degenerate; movement in the branching plane lifts the degeneracy.
2. From a mechanistic point of view, conical intersections often provide the channel mediating radiationless deactivation and photochemical reaction.



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 317

coning and quartering

in analytical chemistry

The reduction in size of a granular or powdered sample by forming a conical heap which is spread out into a circular, flat cake. The cake is divided radially into quarters and two opposite quarters are combined. The other two quarters are discarded. The process is repeated as many times as necessary to obtain the quantity desired for some final use (e.g. as the laboratory sample or as the test sample). If the process is performed only once, coning and quartering is no more efficient than taking alternate portions and discarding the others.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1204

conjugate acid–base pair

The Brønsted acid BH^+ formed on protonation of a base B is called the conjugate acid of B, and B is the conjugate base of BH^+. (The conjugate acid always carries one unit of positive charge more than the base, but the absolute charges of the species are immaterial to the definition.) For example: the Brønsted acid HCl and its conjugate base Cl^- constitute a conjugate acid–base pair.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1099

conjugate solutions

Two solutions that co-exist in equilibrium at a given temperature and pressure and, at constant pressure (temperature), change their compositions and relative proportions with a variation of temperature (pressure). The term usually refers to two immiscible liquids, but it is also applicable to two immiscible solid solutions.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 580

conjugated system (conjugation)

In the original meaning a conjugated system is a molecular entity whose structure may be represented as a system of alternating single and multiple bonds: e.g. $CH_2=CH–CH=CH_2$, $CH_2=CH–C\equiv N$. In such systems, conjugation is the interaction of one p-orbital with another across an intervening σ-bond in such structures. (In appropriate molecular entities d-orbitals may be involved.) The term is

also extended to the analogous interaction involving a p-orbital containing an unshared electron pair, e.g. $:Cl–CH=CH_2$.
See also: delocalization, homoconjugation, resonance

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1099

conjugation

in gene technology

The contact-dependent transfer of a part or all of its genome from one bacterial cell (donor) to another (recipient).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 150

conjugation labelling

in radioanalytical chemistry

Labelling of a substance by conjugation with a labelled molecule.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

conjugative mechanism

See: electronic effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1099

conjunctive name

A name for assemblies of functionalized acyclic parent hydrides and cyclic systems implying the loss of an appropriate number of hydrogen atoms from each.

Source:
Blue Book (Guide), p. 15

connectivity

In a chemical context, the information content of a line formula, but omitting any indication of bond multiplicity.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1099

connectivity

in polymer chemistry

Number of covalent bonds emanating from a constitutional unit of an oligomer molecule or a macromolecule.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1804

consecutive reactions

Also contains definition of: consecutive steps

Reactions occurring in sequence, such as:

$$A \xrightarrow{1} X \xrightarrow{2} Y \xrightarrow{3} Z$$

The overall process is said to occur by consecutive steps.

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 760

conservation of orbital symmetry

The orbital symmetry control of concerted reactions; this requires transformation of the molecular orbitals of reactants into those of products to proceed continuously by following a reaction path along which the symmetry of these orbitals remains unchanged. Reactions which adhere to this requirement are classified as symmetry-allowed reactions, and those which do not as symmetry-forbidden reactions.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1931

consignment

in analytical chemistry

A quantity of material transferred on one occasion and covered by a single set of shipping documents. It may consist of one or more lots or portions of lots. The presence of different lots in a consignment is important from the point of view of the sampling plan and the interpretation of the results of analysis. The term 'population' is used as the general term for the quantity of parent material being sampled when it is immaterial if the parent body is a consignment, lot, batch, entity, etc.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1201

consistency

A general term to describe the property of a material by which it resists permanent change of shape.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

constituent

Chemical species present in a system; often called a component, although the term component has a more restricted meaning in physical chemistry.

Source:
Physical Chemistry Division, unpublished

constitution

The description of the identity and connectivity (and corresponding bond multiplicities) of the atoms in a molecular entity (omitting any distinction arising from their spatial arrangement).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2204
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1100

constitutional heterogeneity

of polymers

The variation in constitution from molecule to molecule in polymers with molecules uniform with respect to elemental composition. An example is a polymer composed of linear and branched molecules; another example is a statistical copolymer comprising two isomeric constitutional units.

Source:
Purple Book, p. 52

constitutional homosequence

A constitutional sequence which contains constitutional units of only one species and in one sequential arrangement.

Source:
Purple Book, p. 35

constitutional isomerism

Isomerism between structures differing in constitution and described by different line formulae e.g. CH_3OCH_3 and CH_3CH_2OH.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205

constitutional repeating unit (CRU)

in polymers

The smallest constitutional unit the repetition of which constitutes a regular macromolecule, a regular oligomer molecule, a regular block or a regular chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2291

constitutional sequence

Also contains definitions of: diads *in polymers*, tetrads *in polymers*, triads

in polymers

The whole or part of a chain comprising one or more species of constitutional unit(s) in defined sequence.
Note:
Constitutional sequences comprising two constitutional units are termed diads, those comprising three constitutional units triads, and so on. In order of increasing sequence lengths they are called tetrads, pentads, hexads, heptads, octads, nonads, decads, undecads, etc.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2299

constitutional unit

An atom or group of atoms (with pendant atoms or groups, if any) comprising a part of the essential structure of a macromolecule, an oligomer molecule, a block or a chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2291

constitutive enzymes

Enzymes which are produced constitutively by the cell under all physiological conditions. Therefore, they are not controlled by induction or repression.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 150

contact angle

When a liquid does not spread on a substrate (usually a solid), a contact angle (θ) is formed which is defined as the angle between two of the interfaces at the three-phase line of contact. It must always be stated which interfaces are used to define θ. It is often necessary to distinguish between the 'advancing contact angle' (θ_{a}), the 'receding contact angle' (θ_{r}) and the 'equilibrium contact angle' (θ_{e}). When $\theta_{\mathrm{r}} \neq \theta_{\mathrm{a}}$ the system is said to exhibit contact angle hysteresis

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 598

contact corrosion

The enhancement of the corrosion rate of the material with the more negative corrosion cell resulting from the contact between different electron-conducting phases.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 22

contact potential difference (Volta potential difference)

The electric potential difference between one point in the vacuum close to the surface of **M1** and another point in the vacuum close to the surface of **M2**, where **M1** and **M2** are two uncharged metals brought into contact.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1257

contamination

Carry-over from a preceding sample probe into a following specimen cup, which will influence not just one result, but all assays on that specimen, or with that reagent.

Source:
PAC, 1991, *63*, 301 *(Proposals for the description and measurement of carry-over effects in clinical chemistry (Recommendations 1991))* on page 302

content

See: substance content

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 967

continuity inversion

in solvent extraction

A change in the mutual dispersion of two phases in contact.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2386

continuous analyser

An analyser in which subassemblies operate continuously.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

continuous bed packing

in liquid chromatography

A column packing, which is a single entity, rather than being composed of individual particles.

Source:
PAC, 1997, *69*, 1475 *(Classification and characterization of stationary phases for liquid chromatography: Part I. Descriptive terminology (IUPAC Recommendations 1997))* on page 1477

continuous flow

See: transport

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

continuous flow enthalpimetry

A term used to describe methods wherein a reagent is continuously fed into a flowing analyte stream and the temperature difference is measured before and after a reactor (mixing chamber). Alternatively, the temperature may be measured in a differential manner between a reference and a reactor chamber. The analyte concentration is directly proportional to the measured temperature difference. Synonymous with continuous flow enthalpimetric analysis.

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2491

continuous indication analyser

An analysis with a permanent indication related to the sample concentration. To obtain a continuous indication, the sampling and measuring cell need to be continuous. A time lag may exist between sampling and indication of measured concentration.
See: dead time of analyser

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

continuous measuring cell

A measuring cell which operates continuously.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2178

continuous operation

in analysis

The operation of an analytical instrument in such a way that no analytical procedure needs to be completed on any sample before the next procedure can be started.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

continuous precipitation

A diffusional reaction in a multi-component system in which atoms are transported to the growing nuclei by diffusion over relatively large distances in the parent phase and during which the mean composition of the parent phase changes continuously towards its equilibrium value. Synonymous with nucleation and growth.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 580

continuous wave (CW) laser

CW operation of a laser means that the laser is continuously pumped and continuously emits electromagnetic radiation. The emission can occur in a single cavity mode or on multiple modes.
Note:
Some lasers are called CW mode-locked. This indicates that the pulse average power is constant, i.e., there is no Q-switched mode locking.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 318

continuous-flow cell

in spectrochemical analysis

A cell which allows liquid (or gaseous) samples to pass through the cell continuously while absorption measurements are made.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1454

contour length **[obsolete]**

in polymers

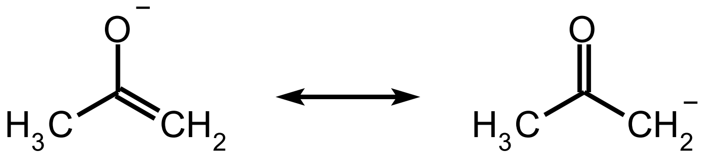
The maximum end-to-end distance of a linear polymer chain. For a single-strand polymer molecule, this usually means the end-to-end distance of the chain extended to the all-*trans* conformation. For chains with complex structure, only an approximate value of the contour length may be accessible. The sum of the lengths of all skeletal bonds of a single-strand polymer molecule is occasionally termed 'contour length'. This use of this term is discouraged.

Source:
Purple Book, p. 50

contributing structure

Also contains definition of: canonical form

The definition is based on the valence-bond formulation of the quantum mechanical idea of the wavefunction of a molecule as composed of a linear combination of wavefunctions, each representative of a formula containing bonds that are only single, double or triple with a particular pairing of electron spins. Each such formula represents a contributing structure, also called 'resonance structure' to the total wavefunction, and the degree to which each contributes is indicated by the square of its coefficient in the linear combination. The contributing structures, also called 'canonical forms', themselves thus have a purely formal significance: they are the components from which wavefunctions can be built. Structures may be covalent (or non-polar) or ionic (or polar). The representation is frequently kept qualitative so that we speak of important or major contributing structures and minor contributing structures. For example, two major non-equivalent contributing structures for the conjugate base of acetone are:



See also: delocalization, Kekulé structure, resonance

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1100

control material

in analysis

A material to be used for the assessment of the performance of an analytical procedure or part thereof.
See: calibration material

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

control sample

in analysis

The test portion or test solution used for assessment of the performance of an analytical procedure.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

controlled atmosphere

in atmospheric chemistry

A synthetic gaseous sample of pure air which may contain carefully determined amounts of certain contaminants; this may be used as a standard for the calibration of analytical techniques, as a simulated environment for the study of biological responses, or for other purposes.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2182

convection (as applied to air motion)

Vertical motion of the air induced by the expansion of the air heated by the earth's surface and its resulting buoyancy.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2182

convenience sample

A sample chosen on the basis of accessibility, expediency, cost, efficiency or other reason not directly concerned with sampling parameters.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1203

conventional transition-state theory

See: transition-state theory

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 162

conventional true value

Value attributed to a particular quantity and accepted, sometimes by convention, as having an uncertainty appropriate for a given purpose. Examples are the CODATA recommended values of fundamental physical constants.

Source:
VIM
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 162

conversion cross-section

Product of the quantum yield by the absorption cross-section, $\sigma\, \Phi$. SI unit is m^2; commonly expressed in cm^2.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 318

conversion electron

Electron ejected from the atom in the process of internal conversion.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

conversion spectrum

A plot of a quantity related to the absorption (absorbance, cross section, etc.) multiplied by the quantum yield for the considered process against a suitable measure of photon energy, such as frequency, ν, wavenumber, σ, or wavelength, λ, e.g. the conversion cross section, $\sigma\varphi$, has the SI unit m^2.
See also: action spectrum, efficiency spectrum, spectral effectiveness

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2234

convex isotherm

in chromatography

Distribution isotherm, the slope of which is continuously decreasing.
Note:
The resulting chromatographic peak is tailing. Adsorption isotherms are often of this type. A special case is the Langmuir adsorption isotherm.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1593

cooperative transition

A transition that involves a simultaneous, collective displacement or change of state of the atoms and/or electrons in the entire system. Examples: An order-disorder transition of atoms or electrons, as in an alloy, a ferromagnet or superconductor; a Jahn–Teller or ferroic transition; a martensitic transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 580

cooperativity

Interaction between the substrate binding sites of an allosteric enzyme. Binding of a substrate molecule to one binding site changes the affinity of the binding sites on the other subunits (cf. allosteric enzymes) to the substrate by induction of a conformation change at the other binding sites. Cooperative enzymes typically display a sigmoid (S-shaped) plot of the reaction rate against substrate concentration.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 151

coordinate covalence [obsolete]

See: coordination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1100

coordinate link [obsolete]

See: coordination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1100

coordination

The formation of a covalent bond, the two shared electrons of which have come from only one of the two parts of the molecular entity linked by it, as in the reaction of a Lewis acid and a Lewis base to form a Lewis adduct; alternatively, the bonding formed in this way. In the former sense, it is the reverse of unimolecular heterolysis. 'Coordinate covalence' and 'coordinate link' are synonymous (obsolescent) terms. The synonym 'dative bond' is obsolete. (The origin of the bonding electrons has by itself no bearing on the character of the bond formed. Thus, the formation of methyl chloride from a methyl cation and a chloride ion involves coordination; the resultant bond obviously differs in no way from the C–Cl bond in methyl chloride formed by any other path, e.g. by colligation of a methyl radical and a chlorine atom.) The term is also used to describe the number of ligands around a central atom without necessarily implying two-electron bonds.
See also: dipolar bond, π-adduct

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1100

coordination entity

An assembly consisting of a central atom (usually metallic) to which is attached a surrounding array of other groups of atoms (ligands).

Source:
Red Book, p. 145

coordination number

1. The coordination number of a specified atom in a chemical species is the number of other atoms directly linked to that specified atom. For example, the coordination number of carbon in methane is four, and it is five in protonated methane, CH_5^+. (The term is used in a different sense in the crystallographic description of ionic crystals.)

   Source:
   PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1100
2. In an inorganic coordination entity, the number of σ-bonds between ligands and the central atom. π-bonds are not considered in determining the coordination number.

Source:
Red Book, p. 146

coordination polyhedron (polygon)

In a coordination entity, the solid figure defined by the positions of the ligand atoms directly attached to the central atom.

Source:
Red Book, p. 146

coordinatively saturated complex

A transition metal complex that has formally 18 outer shell electrons at the central metal atom.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1100

coordinatively unsaturated complex

A transition metal complex that possesses fewer ligands than exist in the coordinatively saturated complex. These complexes usually have fewer than 18 outer shell electrons at the central metal atom.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1100

copolymer

Also contains definitions of: bipolymer, quaterpolymer, terpolymer

A polymer derived from more than one species of monomer.
Note:

Copolymers that are obtained by copolymerization of two monomer species are sometimes termed bipolymers, those obtained from three monomers terpolymers, those obtained from four monomers quaterpolymers, etc.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2300

copolymer micelle

A micelle formed by one or more block or graft copolymer molecules in a selective solvent.

Source:
Purple Book, p. 52

copolymerization

Polymerization in which a copolymer is formed.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2306

copper vapour laser

A pulsed source of coherent radiation emitting at $578.2\ \mathrm{nm}$ and $510.5\ \mathrm{nm}$ from excited copper atoms.
See: gas lasers, laser

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2234

coprecipitation

The simultaneous precipitation of a normally soluble component with a macro-component from the same solution by the formation of mixed crystals, by adsorption, occlusion or mechanical entrapment.

Source:
Orange Book, p. 86

See also:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1199

copy number

in biotechnology

The number of copies of a plasmid or a gene within a cell.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 151

core atom

in organic reaction mechanisms

The primary reference atom in a mechanistic change; usually either of the two atoms of a transformed multiple bond or the single atom at which substitution occurs.

Source:
PAC, 1989, *61*, 23 *(System for symbolic representation of reaction mechanisms (Recommendations 1988))* on page 55

coronands (coronates)

See: crown

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1100

corrected emission spectrum

Obtained after correcting for instrumental and sample effects and usually represented by a graph of Φ_λ against wavelength, where Φ_λ is the spectral (radiant) energy flux.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 242

corrected excitation spectrum

Obtained if the photon flux incident on the sample is held constant. If the solution is sufficiently dilute that the fraction of the exciting radiation absorbed is proportional to the absorption coefficient of the analyte, and if the quantum yield is independent of the exciting wavelength, the corrected excitation spectrum will be identical in shape to the absorption spectrum.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 242

corrected retention volume

in gas chromatography

The corrected retention volume, V_R^0, is given by

$$V_R^0 = j\,V_R$$

where j is the pressure gradient correction factor for a homogeneously filled column of constant diameter and V_R is the retention volume. This quantity is of limited use because it is influenced by the volumes of the sample injector and detector, as well as the interstitial volume of the column.

Source:
Orange Book, p. 104

correlation analysis

The use of empirical correlations relating one body of experimental data to another, with the objective of finding quantitative estimates of the factors underlying the phenomena involved. Correlation analysis in organic chemistry often uses linear free-energy relations for rates or equilibria of reactions, but the term also embraces similar analysis of physical (most commonly spectroscopic) properties and of biological activity.
See also: quantitative structure-activity relationships (QSAR)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1101

correlation coefficient

A measure of the degree of interrelationship which exists between two measured quantities, x and y; the correlation coefficient (r) is defined by the following relation:

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})\,(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

where x_i and y_i are the measured values in the ith experiment of n total experiments, $\bar{x}$ and $\bar{y}$ are the arithmetic means of x_i and y_i:

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}$$

(similar expression for $\bar{y}$). The linear correlation coefficient indicates the degree to which two quantities are linearly related. If $x = a\,y$ is followed then $r = 1$, and departures from this relationship decrease r; if interpretations of data based on the linear correlation coefficient are to be made, one should consult a book on statistics.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2182

correlation diagram

A diagram which shows the relative energies of orbitals, configurations, valence bond structures, or states of reactants and products of a reaction, as a function of the molecular geometry, or another suitable parameter. An example involves the interpolation between the energies obtained for the united atoms and the values for the separated atoms limits.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2234

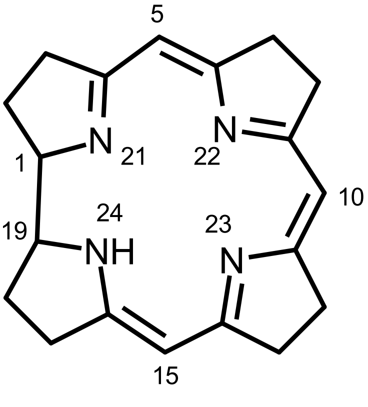
correlation energy

The difference between the Hartree–Fock energy calculated for a system and the exact non-relativistic energy of that system. The correlation energy arises from the approximate representation of the electron-electron repulsions in the Hartree–Fock method.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2234

corrinoids (cobalamines, corphyrins, corrins, vitamin B12 compounds)

Derivatives of the corrin nucleus, which contains four reduced or partly reduced pyrrole rings joined in a macrocycle by three $=\mathrm{CH}-$ groups and one direct carbon–carbon bond linking α positions.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328

See also:
White Book, p. 272

corrosion

An irreversible interfacial reaction of a material (metal, ceramic, polymer) with its enviroment which results in consumption of the material or in dissolution into the material of a component of the enviroment. Often, but not necessarily, corrosion results in effects detrimental to the usage of the material considered. Exclusively physical or mechanical processes such as melting or evaporation, abrasion or mechanical fracture are not included in the term corrosion.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 20

corrosion cell

A galvanic cell resulting from inhomogeneities in the material or in its environment.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 22

corrosion potential, E_{cor}

The electrode potential spontaneously acquired by a corroding material in a particular environment.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 20

corrosion rate

Also contains definition of: corrosion current

The amount of substance transferred per unit time at a specified surface. Using Faraday's law, the corrosion rate, v_{cor}, can be formally expressed as an electric current which at the corrosion potential is called the corrosion current, I_{cor}, e.g. for the anodic dissolution of one component of a material with v_{cor} in $\mathrm{mol\ s^{-1}}$ and I_{cor} in A one obtains $I_{\mathrm{cor}} = n\,F\,v_{\mathrm{cor}}$, n being the charge number of the electrode reaction and F the Faraday constant.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 20

cotectic

The conditions of pressure, temperature and composition under which two or more solid phases crystallize at the same time from a single liquid over a finite range of decreasing temperature.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 580

coulomb

SI derived unit of electric charge, $\mathrm{C} = \mathrm{A{\cdot}s}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 967

coulomb integral, H_{rr}

Integral over space of the type $\int \psi_r{*}\, \hat{H}\, \psi_r \mathrm{d}\tau$ where $\hat{H}$ is the hamiltonian operator containing electrostatic potential energy terms and ψ is a one-electron wavefunction.

Source:
Green Book, 2nd ed., p. 17

Coulomb repulsion

The potential energy component corresponding to the electrostatic interaction between each pair of charged particles:

$$V = \frac{1}{4\,\pi\,\varepsilon_0} \sum_i \sum_{j<i} e_i\, e_j\, \Delta r_{ij}$$

where ε_0 is the permittivity of a vacuum, Δr_{ij} is the distance between the two particles, and e_i and e_j are the charges on particles i and j. In molecular orbital theory, the electrostatic repulsion between the two electrons occupying the orbitals Ψ_i and Ψ_j. In the Hartree–Fock method, the mean Coulomb repulsion is determined by the value of the Coulomb integral

$$J_{ij} = \int\int \Psi_{i*}(\mathbf{r}_1)\, \Psi_i(\mathbf{r}_1) \left(\frac{e^2}{r_{12}}\right) \Psi_{j*}(\mathbf{r}_2)\, \Psi_j(\mathbf{r}_2) \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 = \, < ij \mid ij >$$

See also: exchange repulsion

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1932

coulometric detection method

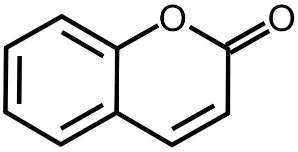
in electrochemical analysis

A detection method in which the current is directly proportional to the flow rate of the substance involved in the electrochemical reaction, and the amount of charge which flows is proportional to the amount of substances taking part in the reaction.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

coumarins

2*H*-Chromen-2-one (older name 1,2-benzopyrone), trivially named coumarin, and its derivatives formed by substitution.



See: isocoumarins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328

count

1. Information corresponding to a pulse processed for counting.
2. Number of pulses recorded during a measurement.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

counter tube

Radiation detector consisting of a gas-filled tube or valve whose gas amplification is much greater than one, and in which the individual ionizing events give rise to discrete electrical pulses. Often an expression is added indicating the geometry (e.g. end window), composition of the gas (e.g. helium) or the physical process for its operation (e.g. proton recoil, fission).

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

counter-current flow

Flow through a membrane module in which the fluids on the upstream and downstream sides of the membrane move parallel to the membrane surface but in opposite directions.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1481

counter-ions

1. (*in an ion exchanger*) the mobile exchangeable ions.

   Source:
   PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 854
2. (*in colloid chemistry*) ions of low relative molecular mass, with a charge opposite to that of the colloidal ion.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

counting efficiency

Synonym: efficiency
of a counter

The ratio between the number of particles or photons counted with a radiation counter and the number of particles or photons of the same type and energy emitted by the radiation source.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517

counting loss

A reduction of the counting rate resulting from phenomena such as the resolving time or the dead time.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517
Orange Book, p. 217

counting rate

The number of counts occuring in unit time.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517

coupled cluster (CC) method

A method employed in *ab initio* quantum mechanical calculations providing for a higher-level treatment of electron correlation beyond MP4.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1932

coupled (indicator) reaction

Synonym: indicator reaction

in analysis

A reaction which follows the (slower) reaction of kinetic interest, so as to provide means of monitoring the formation of a reaction product. This reaction is sometimes referred to as the indicator reaction.

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2294

coupled simultaneous techniques

in analysis

The application of two or more techniques to the same sample when the two instruments involved are connected through an interface, e.g. simultaneous thermal analysis and mass spectrometry.

Source:
Orange Book, p. 39

coupling constant (spin-spin), J

A quantitative measure for nuclear spin-spin, nuclear-electron (hyperfine coupling) and electron-electron (fine coupling in EPR) coupling in magnetic resonance spectroscopy. The 'indirect' or scalar NMR coupling constants are in a first approximation independent of the external magnetic field and are expressed in Hz.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1101

covalent bond

A region of relatively high electron density between nuclei which arises at least partly from sharing of electrons and gives rise to an attractive force and characteristic internuclear distance.

See also: agostic, coordination, hydrogen bond, multi-centre bond

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1101

Cox–Yates equation

A modification of the Bunnett–Olsen equation of the form:

$$\log_{10}\left(\frac{[\mathrm{SH}^+]}{[\mathrm{S}]}\right) - \log_{10}[\mathrm{H}^+] = m^* X + \mathrm{pK}_{\mathrm{SH}^+}$$

is the activity function

$$\log_{10}\left(\frac{\gamma_{\mathrm{S}}\,\gamma_{\mathrm{H}^+}}{\gamma_{\mathrm{SH}^+}}\right)$$

for an arbitrary reference base. The function X is called the excess acidity because it gives a measure of the difference between the acidity of a solution and that of an ideal solution of the same concentration. In practice

$$X = -(\mathrm{H}_0 + \log_{10}[\mathrm{H}^+])$$

and

$$m^* = 1 - \Phi.$$

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1101

cracking

Also contains definition of: hydrocarbon cracking

The thermal or catalytic decomposition of a compound such as a hydrocarbon into chemical species of smaller molecular weight.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

crazing

Formation of cavities, when a polymer is stressed, which contain load-bearing fibrils spanning the gap between the surfaces of each cavity.

Source:
PAC, 1996, *68*, 2313 *(Definitions of terms relating to degradation, aging, and related chemical transformations of polymers (IUPAC Recommendations 1996))* on page 2317

cream

A highly concentrated emulsion formed by creaming of a dilute emulsion.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 611

cream volume

The volume of cream formed in an emulsion.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 616

creaming

The macroscopic separation of a dilute emulsion into a highly concentrated emulsion, in which interglobular contact is important, and a continuous phase under the action of gravity or a centrifugal field. This separation usually occurs upward, but the term may still be applied if the relative densities of the dispersed and continuous phases are such that the concentrated emulsion settles downward.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 611

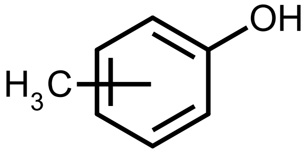
creep

Time-dependent change of the dimensions of a material under a constant load.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1810

cresols

The monomethylphenols and their derivatives formed by substitution on the ring with substituents other than –OH.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328

critical energy (threshold energy)

A chemical reaction cannot occur, except by quantum-mechanical tunnelling unless the total energy available is greater than a certain energy, which is known as the critical energy, or the threshold energy.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 162

critical excitation energy, E_q

in in situ microanalysis

Minimum energy to excite a specific analytical signal. The term is most frequently used in connection with the generation of X-ray spectra, designating the ionization (binding) energy of the orbital on which the transition ends.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2027

critical ion-concentration in an ionomer

Concentration of ionic groups in an ionomer matrix above which ionic aggregation occurs.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2069

critical micelle concentration

Acronym: cmc

There is a relatively small range of concentrations separating the limit below which virtually no micelles are detected and the limit above which virtually all additional surfactant molecules form micelles. Many properties of surfactant solutions, if plotted against the concentration, appear to change at a different rate above and below this range. By extrapolating the loci of such a property above and below this range until they intersect, a value may be obtained known as the critical micellization

concentration (critical micelle concentration), symbol c_M, abbreviation cmc (or c.m.c.). As values obtained using different properties are not quite identical, the method by which the cmc is determined should be clearly stated.
See also: inverted micelle

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1101

critical point

The temperature and pressure at which the liquid and vapour intensive properties (density, heat capacity, etc.) become equal. It is the highest temperature (critical temperature) and pressure (critical pressure) at which both a gaseous and a liquid phase of a given compound can coexist.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183
PAC, 1993, *65*, 2397 *(Nomenclature for supercritical fluid chromatography and extraction (IUPAC Recommendations 1993))* on page 2399

critical pressure, p_c

The minimum pressure which would suffice to liquefy a substance at its critical temperature. Above the critical pressure, increasing the temperature will not cause a fluid to vaporize to give a two-phase system.

Source:
PAC, 1993, *65*, 2397 *(Nomenclature for supercritical fluid chromatography and extraction (IUPAC Recommendations 1993))* on page 2399

critical solution composition

See: critical solution point

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 580

critical solution point

Synonym: consolute point

The point, with coordinates critical solution temperature and critical composition, on a temperature-composition phase diagram at which the distinction between co-existent phases vanishes. In solid-solid, solid-liquid and liquid-liquid systems both upper and lower critical solution temperatures and corresponding critical solution compositions can occur. Synonymous with consolute point.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 580

critical solution temperature

See: critical solution point

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 580

critical study

Investigation yielding the no observed adverse effect level that is used by the USEPA as the basis of the reference dose.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1038

critical temperature, T_c

That temperature, characteristic of each gas, above which it is not possible to liquefy a given gas.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183
PAC, 1993, *65*, 2397 *(Nomenclature for supercritical fluid chromatography and extraction (IUPAC Recommendations 1993))* on page 2399

critical thickness

of a film

A film often thins gradually to a thickness at which it either ruptures or converts abruptly to an equilibrium film. This thickness is sometimes well enough defined statistically to be considered a critical thickness, t_c or h_c.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 614

cross reaction

The ability of substances other than the analyte to bind to the binding reagent and the ability of substances other than the binding reagent to bind the analyte in competitive binding assays.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517

cross-conjugation

In a system XC_6H_4GY this is conjugation involving the substituent X, the benzene ring and the side-chain connective-plus-reaction site GY, i.e. either X is a +*R* group and GY is a -*R* group, or X is a -*R* group and GY is a +*R* group. In Hammett correlations this situation can lead to the need to apply exalted substituent constants σ^{+} or σ^{-}, respectively, as in electrophilic or nucleophilic aromatic substitution, respectively. The term 'through resonance' is synonymous. Cross conjugation has also been used to describe the interactions occurring in 2-phenylallyl and similar systems.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1101

cross-flow filtration

in biotechnology

Method of operating a filtration device where retained fluid is circulated over the membrane (filter) surface thus preventing undue build-up of filtered material on membrane (filter).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 151

cross-over concentration, c^{*}

The concentration range at which the sum of the volumes of the domains occupied by the solute molecules or particles in solution is approximately equal to the total volume of that solution. The term 'domain' refers to the smallest convex body that contains the molecule or particle in its average shape.

Source:
Purple Book, p. 57

crossed electric and magnetic fields

in mass spectrometry

Electric and magnetic fields with the electric field direction at right angles to the magnetic field direction.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1544

crossing over

in biotechnology

The usually reciprocal exchange of genetic material between chromosomes; part of natural genetic recombination.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 151

crosslink

A small region in a macromolecule from which at least four chains emanate, and formed by reactions involving sites or groups on existing macromolecules or by interactions between existing macromolecules.
Notes:

1. The small region may be an atom, a group of atoms, or a number of branch points connected by bonds, groups of atoms, or oligomeric chains.
2. In the majority of cases, a crosslink is a covalent structure but the term is also used to describe sites of weaker chemical interactions, portions of crystallites, and even physical entanglements.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2298

crosslink density

Number of crosslinks per unit volume in a polymer network.
See also: junction-point density

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1819

crosslinking

Reaction involving sites or groups on existing macromolecules or an interaction between existing macromolecules that results in the formation of a small region in a macromolecule from which at least four chains emanate.
Notes:

1. The small region may be an atom, a group of atoms, or a number of branch points connected by bonds, groups of atoms, or oligomeric chains.
2. A reaction of a reactive chain end of a linear macromolecule with an internal reactive site of another linear macromolecule results in the formation of a branch point, but is not regarded as a crosslinking reaction.

See also: crosslink

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1821

crosslinking site

Site on a macromolecule or region in a polymer material that takes part in the formation of chemical or physical crosslinks.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1819

crowding

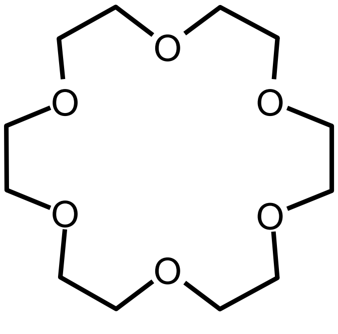
in solvent extraction

The displacement of an impurity from an extract phase by contact with a solution containing the main extractable solute. The main solute need not be present in a pure solution but should have a higher distribution ratio than the impurities present.
See also: scrubbing, exchange extraction

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2386

crown

A molecular entity comprising a monocyclic ligand assembly that contains three or more binding sites held together by covalent bonds and capable of binding a *guest* in a central (or nearly central) position. The adducts formed are sometimes known as 'coronates'. The best known members of this group are macrocyclic polyethers, such as '18-crown-6', containing several repeating units $–CR_2–CR_2O–$ (where R is most commonly H), and known as crown ethers.



18-crown-6

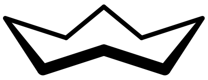
See also: host

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1101

See also:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1328

crown conformation

A conformation of a saturated cyclic molecular entity, containing an even number (≥8) of atoms in the ring, in which these atoms lie alternately in each of two parallel planes and are symmetrically equivalent (D_{4d} for cyclooctane, D_{5d} for cyclodecane etc). It is analogous to the chair conformation of cyclohexane.



See also: tub conformation

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205

crud

in solvent extraction

A deposit or emulsion at the interface between two partially settled phases.
Notes:

1. The phenomenon of crud formation arises from many causes and this definition does not imply any single one.
2. Other terms -- some unprintable -- have been used but crud is the generally accepted term.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2387

cryogenic

Low temperature processes, apparatus, etc.; usually applied to systems operated at the temperature of liquid nitrogen, helium or other condensed gas which boils at a very low temperature (at atmospheric pressure).
See: cryogenic sampling

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

cryogenic sampling

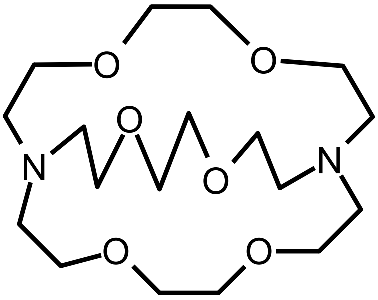
The collection of trace compounds from gaseous media by cocondensation with a major constituent (e.g. water vapour, CO_2, N_2, Ar) of the matrix.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2212

cryptand

Also contains definition of: cryptate

A molecular entity comprising a cyclic or polycyclic assembly of binding sites that contains three or more binding sites held together by covalent bonds, and which defines a molecular cavity in such a way as to bind (and thus 'hide' in the cavity) another molecular entity, the guest (a cation, an anion or a neutral species), more strongly than do the separate parts of the assembly (at the same total concentration of binding sites). The adduct thus formed is called a 'cryptate'. The term is usually restricted to bicyclic or oligocyclic molecular entities. Example:



Corresponding monocyclic ligand assemblies crowns are sometimes included in this group, if they can be considered to define a cavity in which a guest can hide. The terms 'podand' and 'spherand' are used for certain specific ligand assemblies. Coplanar cyclic polydentate ligands, such as porphyrins, are not normally regarded as cryptands.
See also: host

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1102
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1329

crystal diffraction spectrometer

A spectrometer, in which diffraction by a crystal is used to obtain the energy spectra of electromagnetic radiation as well as of slow neutrons.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552

crystal field

The average static electric field experienced by an ion, molecule or atom in a crystal generated by all the other surrounding atoms, molecules, or ions. The concept introduced by Becquerel and developed by Bethe has been extended to refer to the field generated by the ligands (anions or neutral species) surrounding a transition metal ion in a coordination compound. With the understatement that some covalency may exist in the metal-ligand bond, it is often referred to as ligand field.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1932

crystal field splitting

The removal of a degeneracy of the energy levels of molecular entities or ions due to the lower site symmetry created by a crystalline environment. This term is sometimes incorrectly used synonymously with the term ligand field splitting.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2234

crystal laser

A solid state laser in which the active medium is composed of ionic species supported in a crystalline host. The first laser used a ruby crystal in which chromium ions as the active medium were supported in an aluminium oxide (sapphire) crystal. One of the most common crystal lasers involves neodymium atoms in a yttrium aluminium garnet host crystal (the YAG:Nd laser).

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1920

crystal photochemistry

Photochemical process in the crystal lattice of a photoactive compound or of a chromophore in the crystal lattice of host molecules. Often asymmetric photochemistry takes place.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 319

crystalline electrodes

Also contains definitions of: heterogeneous membrane electrode, homogeneous membrane electrode

Electrodes which contain mobile ions of one sign and fixed sites of opposite sign. They may be homogeneous or heterogeneous.

1. Homogeneous membrane electrodes are ion-selective electrodes in which the membrane is a crystalline material prepared from either a single compound or a homogeneous mixture of compounds (i.e. Ag_2S, AgI / Ag_2S).
2. Heterogeneous membrane electrodes are formed when an active substance, or mixture of active substances, is mixed with an inert matrix, such as silicone rubber or PVC, or placed on hydrophobized graphite or conducting epoxy, to form the heterogeneous sensing membrane.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2534

crystalline polymer

A polymer showing crystallinity. One or two-dimensional order leads to mesophase structure. The range of order may be as small as about $2\ \mathrm{nm}$ in one (or more) crystallographic direction(s) and is usually below $50\ \mathrm{nm}$ in at least one direction.

Source:
Purple Book, p. 74

crystallinity

The presence of three-dimensional order on the level of atomic dimensions. Crystallinity may be detected by diffraction techniques, heat-of-fusion measurements, etc. The amount of disorder within the crystalline region is not incompatible with this concept.

Source:
Purple Book, p. 74

crystallization

The formation of a crystalline solid from a solution, melt vapour or a different solid phase, generally by the lowering of the temperature or by evaporation of a solvent.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 580

CT

Abbreviation for charge-transfer.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2234

cumulative double bonds

Those present in a chain in which at least three contiguous carbon atoms are joined by double bonds; non-cumulative double bonds comprise every other arrangement of two or more double bonds in a single structure. The generic name 'cumulene' is given to compounds containing three or more cumulative double bonds.

Source:
Blue Book, p. 20

cumulative fission yield

The fraction of fissions which have resulted in the production of a nuclide either directly or indirectly, up to a specified time. If no time is specified, the yield is considered to be the asymptotic value.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

cumulative sample

A sample collected over an extended period of time.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

cumulenes

Hydrocarbons (and by extension, derivatives formed by substitution) having three or more cumulative double bonds, e.g. $R_2C=C=C=CR_2$.
See also: allenes, heterocumulenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1329

cumulonimbus cloud

in atmospheric chemistry

Heavy masses of dense cloud whose cumuliform summits rise in the forms of towers, the upper parts having a fibrous texture and often spreading out into the shape of an anvil; these clouds generally produce showers of rain and sometimes of snow, hail or soft hail, and often develop into thunderstorms; up to $12\ 000\ \mathrm{m}$; summits may be as cold as $-50\ °\mathrm{C}$; strong convective motions with vertical velocities of 3 to greater than $30\ \mathrm{m\ s^{-1}}$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

cumulus cloud

in atmospheric chemistry

Detached, dense clouds with a dome-shaped upper surface with sharp-edged, rounded protuberances and a nearly horizontal base; $600 - 6000\ \mathrm{m}$ or more; convective motion with rising, large bubbles of warm air with vertical speeds of $1\ - 5\ \mathrm{m\ s^{-1}}$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

cupola

A vertical shaft furnace used for melting metals; the melting of ores is accomplished in a blast furnace.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

curie

Non-SI unit of radioactivity, $\mathrm{Ci} \approx 3.7 \times 10^{10}\ \mathrm{Bq}$.

Source:
Green Book, 2nd ed., p. 113
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 967
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517

curing

Chemical process of converting a prepolymer or a polymer into a polymer of higher molar mass and then into a network.
Notes:

1. Curing is achieved by the induction of chemical reactions which might or might not require mixing with a chemical curing agent.
2. Physical aging, crystallization, physical crosslinking and post-polymerization reactions are sometimes referred to as 'curing'. Use of the term 'curing' to describe such processes is deprecated.

See also: vulcanization

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1822

current density

The current density $\boldsymbol{j}_\mathbf{B}$ of a species **B** in a given point of the solution is obtained by multiplying the flux density of that species at the given point by the Faraday constant F and by the charge number z_B of the species:

$$\boldsymbol{j}_\mathbf{B} = z_\mathrm{B}\, F\, \boldsymbol{N}_\mathbf{B}$$

where $\boldsymbol{j}_\mathbf{B}$ is a vector which indicates the direction in which the charges transported by the species **B** flow and which gives the number of these charges going through a plane oriented perpendicular to the vector, divided by time and by area, and $\boldsymbol{N}_\mathbf{B}$ is the flux density of a minor constituent of the solution with respect to a fixed frame of reference.
See also: electric current density

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1833

current distribution

Also contains definitions of: current density (relative local), primary current distribution, relative local current density, secondary current distribution, tertiary current distribution, throwing power, Wagner number

The ratio of current density at a point X on an interface to the average current density ($\frac{j_\mathrm{x}}{j}$) is called the relative local current density. The current distribution is described by the function $\frac{j_\mathrm{x}}{j} = f(x)$ (or more generally, $\frac{j_\mathrm{x}}{j} = f(x,\, y,\, z)$ where x or $(x,\, y,\, z)$ are the coordinates of the points of the electrode-solution interface. The primary current distribution is that which establishes itself when the influence of overpotential is negligible. The secondary current distribution is that which establishes itself when the influence of the overpotential cannot be neglected but concentration overpotential is negligible. The secondary distribution is often described in terms of dimensionless numbers of the form

$$\mathrm{Wa} = \frac{\kappa}{l}\,\frac{\mathrm{d}\eta}{\mathrm{d}j}$$

where κ is the conductivity of the solution, $\frac{\mathrm{d}\eta}{\mathrm{d}j}$ the slope of the overpotential-current curve under the above conditions and l a characteristic length of the system, for instance the radius of a disc electrode. Wa is the Wagner number. It is a quantity which determines the throwing power and characterizes the equalizing influence of overpotential on the current distribution. In electroplating the throwing power is qualitatively defined as 'the ability of a solution to deposit metal uniformly upon a cathode of irregular shape'. The tertiary current distribution is that which establishes itself when the influence of the overpotential (including concentration overpotential) cannot be neglected.

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1836

current efficiency

Also contains definition of: metal distribution

If several reactions take place simultaneously at the electrode a partial electrode current density (c.d.) j_k can be assigned to each reaction. It is given by the stoichiometry of the reaction and by the amount of substance of **B** reacting (per unit time and per unit electrode area) in the reaction considered. The current efficiency of reaction k, ε_k is defined as the ratio of j_k to the total c.d.:

$$\varepsilon_k = \frac{j_k}{\sum_m j_m}$$

Note that ε_k may be larger than one if cathodic and anodic reactions take place simultaneously at the same electrode. However, ε_k still gives correctly the product yield, which is the quantity of industrial interest. The product yield is the amount of substance of **B** produced per unit charge and is equal to $\frac{\varepsilon_k \nu_{B,k}}{n_k F}$ (in the absence of a chemical reaction which is consecutive to the electrode reaction and which consumes or produces species B). n_k is the charge number of electrode reaction k. Note that in the case of simultaneous electrode reactions the distribution of the partial c.d. j_k may be different from that of the total c.d., i.e. the function $\frac{(j_k)_x}{j} = f_k(x)$ may be different from $\frac{j_x}{j} = f(x)$. In electroplating the term 'metal distribution' is sometimes used to designate the distribution $f_k(x)$ of the partial c.d. for metal deposition.

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1836

current migration

See: migration current

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1497

current yield

See: photocurrent yield

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2234

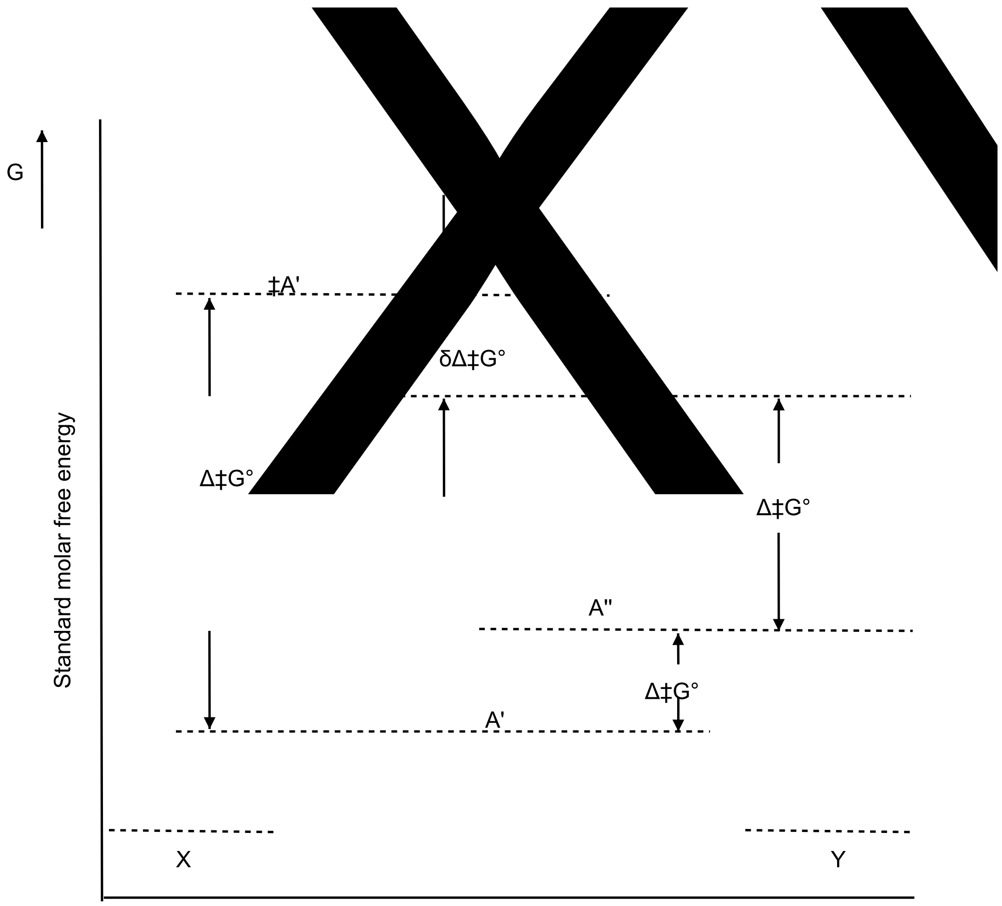
Curtin–Hammett principle

In a chemical reaction that yields one product (X) from one conformational isomer (A') and a different product (Y) from another conformational isomer (A'') (and provided these two isomers are rapidly interconvertible relative to the rate of product formation, whereas the products do not undergo interconversion) the product composition is not in direct proportion to the relative concentrations of the conformational isomers in the substrate ; it is controlled only by the difference in standard free energies ($\delta\Delta^{\ddagger}G$) of the respective transition states.

$$\mathrm{X} \xleftarrow{k_{\mathrm{X}}} \mathrm{A'} \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} \mathrm{A''} \xrightarrow{k_{\mathrm{Y}}} \mathrm{Y}$$

$$k_1 >> k_{\mathrm{X}} \qquad k_{-1} >> k_{\mathrm{Y}}$$

It is also true that the product composition is formally related to the relative concentrations of the conformational isomers A' and A'' (i.e. the conformational equilibrium constant) and the respective rate constants of their reactions; these parameters are generally — though not invariably — unknown. The diagram below represents the energetic situation for transformation of interconverting isomers A and A' into products X and Y.



Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1102

curve-crossing model

Model of organic reactivity that generates a reaction profile from curves that describe the energies of reactant, product, and intermediate electronic configurations (or, alternatively, reactant, product and intermediate electronic states) as a function of the reaction coordinate. The crossing reflects the electronic reorganization that accompanies the transformation of reactants and products.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1933

cut off

in aerosol sizes

in atmospheric chemistry

The size of particles at which the retention efficiency of an instrument device drops below a specified value under defined conditions.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

cut-off filter

An optical device which only permits the transmission of radiation of wavelengths that are longer than or shorter than a specified wavelength. Usually, the term refers to devices which transmit radiation of wavelengths longer than the specified wavelength.
See: filter

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2234

cut-on filter

Optical device that only permits the transmission of radiation of wavelengths shorter than a specified wavelength.
Note:
Although more rare than the cut-off filters, there are a few cut-on filters on the market.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 319

CW

Abbreviation for continuous wave, i.e. non-pulsed source of electromagnetic radiation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2234

cyanates

Salts and esters of cyanic acid, $HOC{\equiv}N$, e.g. KOCN potassium cyanate, PhOCN phenyl cyanate.
See: isocyanates

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1329

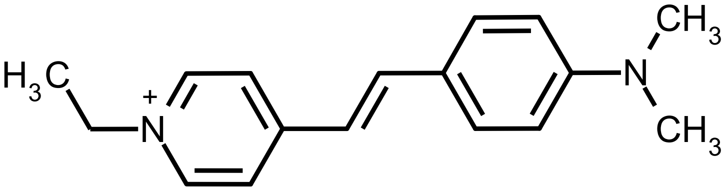
cyanides

Salts and *C*-organyl derivatives of hydrogen cyanide, $HC{\equiv}N$, e.g. $CH_3C{\equiv}N$ methyl cyanide (acetonitrile), NaCN sodium cyanide, PhC(=O)CN benzoyl cyanide.
See also: isocyanides, nitriles, carbonitriles

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1329

cyanine dyes

Synthetic dyes with the general formula $R_2N[CH{=}CH]_nCH{=}N^+R_2 \longleftrightarrow R_2N^+{=}CH[CH{=}CH]_nNR_2$ (*n* is a small number) in which the nitrogen and part of the conjugated chain usually form part of a heterocyclic system, such as imidazole, pyridine, pyrrole, quinoline and thiazole, e.g.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1329

cyanogenic

Compounds able to produce cyanide; examples are the cyanogenic glycosides such as amygdalin in peach and apricot stones.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2035

cyanohydrins

Alcohols substituted by a cyano group, most commonly, but not limited to, examples having a cyano and a hydroxy group attached to the same carbon atom, formally derived from aldehydes or ketones by the addition of hydrogen cyanide. An individual cyanohydrin can systematically be named as a hydroxy nitrile, e.g. $(CH_3)_2C(OH)C{\equiv}N$ 'acetone cyanohydrin' (2-hydroxy-2-methylpropanenitrile), $HOCH_2CH_2C{\equiv}N$ 'ethylene cyanohydrin' (3-hydroxypropanenitrile).
See: halohydrins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1329

cybotactic region

Also contains definition of: cosphere

That part of a solution in the vicinity of a solute molecule in which the ordering of the solvent molecules is modified by the presence of the solute molecule. The term solvent 'cosphere' of the solute has also been used.
See also: solvation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1103

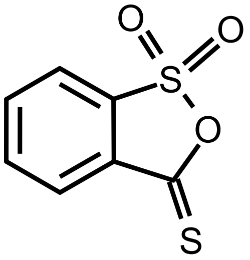
cycles per second

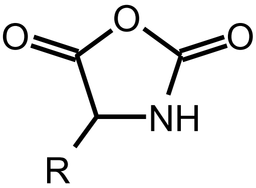
See: hertz

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 967

cyclic acid anhydrides (cyclic anhydrides)

Acid anhydrides derived by loss of water between two oxoacid functions $R_kE(=O)_l(OH)_m$ ($l \neq 0$) (carboxylic, sulfonic, etc.) in the same molecule so as to close a ring. Oxo oxygen replacement analogues are included, e.g.





See: thioanhydrides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1329

cyclitols

Hydroxylated cycloalkanes containing at least three hydroxy groups, each attached to a different ring carbon atom.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1330

White Book, p. 196

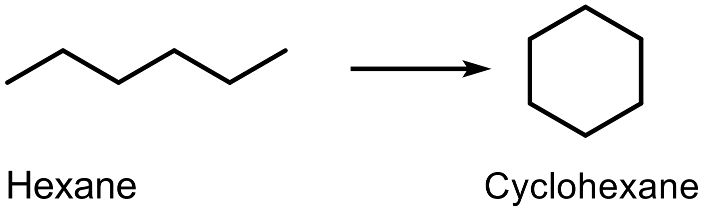
cyclization

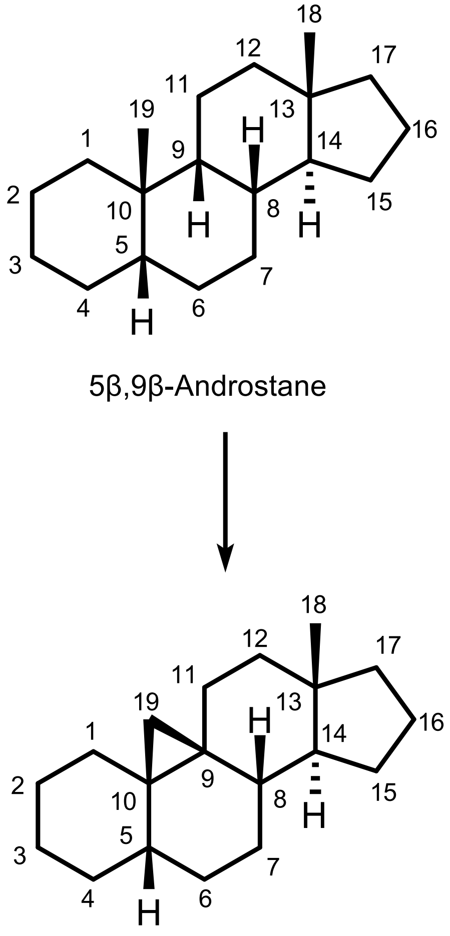
Formation of a ring compound from a chain by formation of a new bond.
See also: annulation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1103

cyclo-

1. A prefix used in names to designate a ring structure, usually italicized in inorganic, but not in organic nomenclature. Examples:




5β,9β-Androstane

9,19-Cyclo-5β,9β-androstane

Source:
Red Book, p. 245
Blue Book, p. 497

See also:
Blue Book (Guide), p. 30

2. The prefix for an elementary reaction or some part thereof indicating that the bonds undergoing primitive changes form part of a ring in the transition state of a pericyclic process.

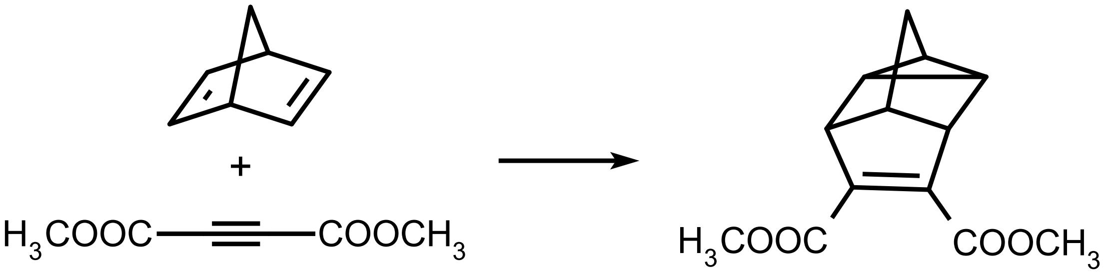
   Source:
   PAC, 1989, *61*, 23 *(System for symbolic representation of reaction mechanisms (Recommendations 1988))* on page 34

cycloaddition

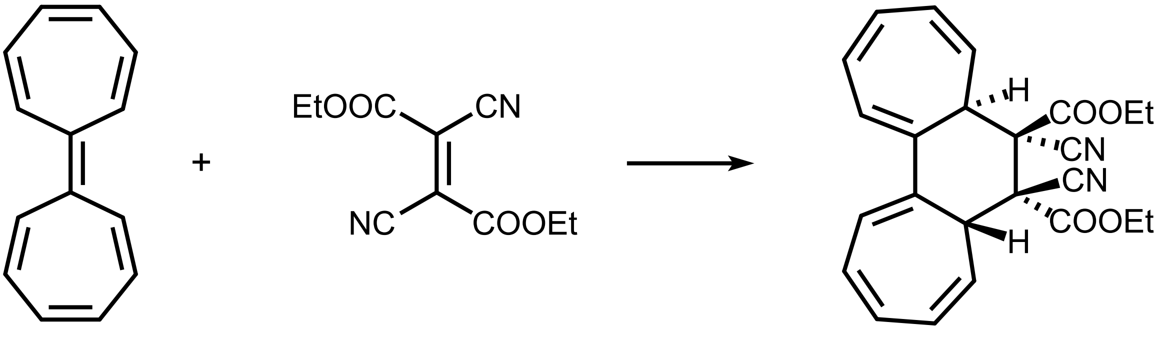
Also contains definition of: dipolar cycloaddition

A reaction in which two or more unsaturated molecules (or parts of the same molecule) combine with the formation of a cyclic adduct in which there is a net reduction of the bond multiplicity. The following two systems of notations have been used for the more detailed specification of cycloadditions, of which the second, more recent system [described under (2)] is preferred:

1. A($i + j + ...$) cycloaddition is a reaction in which two or more molecules (or parts of the same molecule), respectively, provide units of i, j, ... linearly connected atoms: these units become joined at their respective termini by new σ-bonds so as to form a cycle containing ($i + j + ...$) atoms. In this notation, (a) a Diels–Alder reaction is a (4+2) cycloaddition, (b) the initial reaction of ozone with an alkene is a (3+2) cycloaddition, and (c) the reaction shown below is a (2+2+2) cycloaddition. (N.B.: parentheses (...) are used in the description based on numbers of atoms.)



2. The symbolism [$i + j + ...$] for a cycloaddition identifies the numbers i, j, ... of electrons in the interacting units that participate in the transformation of reactants to products. In this notation the reaction (a) and (b) of the preceding paragraph would both be described as [2+4] cycloadditions, and (c) as a [2+2+2] cycloaddition. The symbol a or s (a = antarafacial, s = suprafacial) is often added (usually as a subscript after the number to designate the stereochemistry of addition to each fragment. A subscript specifying the orbitals, *viz.* σ, π (sigma, pi) with their usual significance) or n (for an orbital associated with a single atom only), may be added as a subscript before the number. Thus the normal Diels–Alder reaction is a [$4_s + 2_s$] or [${}_{\pi}4_s + {}_{\pi}2_s$] cycloaddition, whilst the reaction:



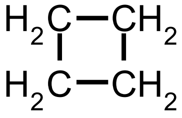
would be a [$14_a + 2_s$] or [${}_{\pi}14_a + {}_{\pi}2_s$] cycloaddition. (N.B. Square brackets [...] are used in the descriptions based on numbers of electrons.) Cycloadditions may be pericyclic reactions or (non-concerted stepwise reactions . The term 'dipolar cycloaddition' is used for cycloadditions of 1,3-dipolar compounds.

See also: cheletropic reactions

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1103

cycloalkanes

Saturated monocyclic hydrocarbons (with or without side chains), e.g. cyclobutane. Unsaturated monocyclic hydrocarbons having one endocyclic double or one triple bond are called cycloalkenes and cycloalkynes, respectively. Those having more than one such multiple bond are cycloalkadienes, cycloalkatrienes, etc. The inclusive terms for any cyclic hydrocarbons having any number of such multiple bonds are cyclic olefins or cyclic acetylenes.

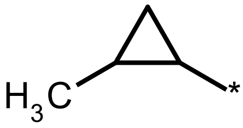


See: alicyclic compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1330

cycloalkyl groups

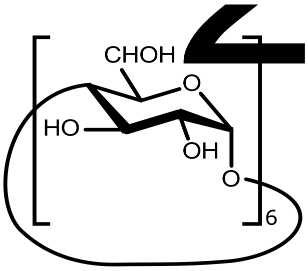
Univalent groups derived from cycloalkanes by removal of a hydrogen atom from a ring carbon atom, e.g. 2-methylcyclopropyl.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1330

cyclodextrins

Cyclic oligoglucosides containing 5 to *ca*. 10 glucose residues in which an enclosed tubular space allows reception of a guest molecule to form a clathrate. The synonymous term Schardinger dextrins is not recommended. (α-Cyclodextrin has 6 glucose residues; β-cyclodextrin has 7.) Semi-systematically α-cyclodextrin is called cyclomaltohexaose.



See also: dextrins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1330

cycloelimination

Synonym: cycloreversion

The reverse of cycloaddition. The term is preferred to the synonyms 'cycloreversion', 'retro-addition' and 'retrocycloaddition'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1104

cyclohexadienyl cations

A subclass of arenium ions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1330

cyclone (collector)

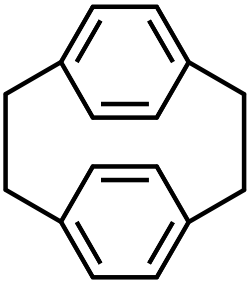
in atmospheric chemistry

A dust, grit or droplet separator utilizing essentially the centrifugal force derived from the motion of the gas. The flow of gases containing suspended particles into the device is transformed into a confined vortex from which centrifugal forces tend to drive the suspended particles to the wall of the cyclone body. The agglomerated particles are subsequently removed from the cyclone by gravitational action.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

cyclophanes

The term originally applied to compounds having two *p*-phenylene groups held face to face by $–[CH_2]_n–$ bridges. It now designates compounds having (i) mancude-ring systems, or assemblies of mancude-ring systems, and (ii) atoms and/or saturated or unsaturated chains as alternate components of a large ring. E.g. [2.2](1,4)(1,4)cyclophane [or 1(1,4),4(1,4)-dibenzenacyclohexaphane].



Many chemists include in this class any bridged aromatic system, irrespective of the attachment positions of the bridge.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1330

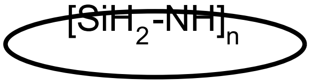
cyclopolymerization

A polymerization in which the number of cyclic structures in the constitutional units of the resulting macromolecules is larger than in the monomer molecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2306

cyclosilazanes

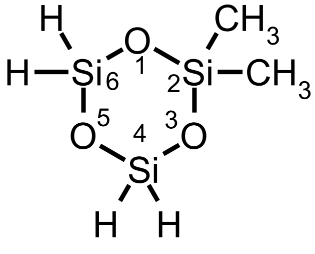
Compounds having rings of alternating silicon and nitrogen atoms:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1330

cyclosiloxanes

Compounds having rings of alternating silicon and oxygen atoms, e.g. 2,2-dimethylcyclotrisiloxane.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1330

cyclotron

A particle accelerator in which the particles travel in a succession of semicircular orbits of increasing radii under the influence of a magnetic field and are accelerated at the beginning of each such orbit by traversing an electric field produced by a high-frequency generator.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1539

cytochrome P450

Member of a superfamily of heme-containing monooxygenases involved in xenobiotic metabolism, cholesterol biosynthesis, and steroidogenesis, in eukaryotic organisms found mainly in the endoplasmic reticulum and inner mitochondrial membrane of cells. ‘P450’ refers to a feature in the carbon monoxide absorption difference spectrum at $450\ \mathrm{nm}$ caused by the presence of a thiolate in the axial position of the heme opposite to the carbon monoxide ligand.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1048

cytochromes

Conjugated proteins containing haem as the prosthetic group and associated with electron transport and with redox processes. The terminal electron transport chain of oxidative respiration contains at least five different cytochromes.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 151

Δ (delta), Λ (lambda)

Designations of stereoisomers of tris(didentate) metal complexes and other octahedral complexes.
See: helicity

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205
Red Book, p. 184

D, L, DL

See: Fischer–Rosanoff convention

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205

d, l, dl [obsolete]

Obsolete (usage strongly discouraged) alternatives for, respectively, the prefixes (+)- and (−)- [used to designate the sign of optical rotation of enantiomers under specified condition (and hence to distinguish the enantiomers)] and (±)- for a racemate.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205

3D-QSAR (three-dimensional quantitative structure–activity relationships)

Three-dimensional quantitative structure-activity relationships (3D-QSAR) involve the analysis of the quantitative relationship between the biological activity of a set of compounds and their three-dimensional properties using statistical correlation methods.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1142

dalton

Non-SI unit of mass (symbol Da), equal to the unified atomic mass unit (atomic mass constant). It is often used in biochemistry and molecular biology although it was never approved by the Conférence Général des Poids et Mesures.

Source:
Green Book, 2nd ed., p. 111
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 968

dark photochemistry (photochemistry without light) [obsolete]

Chemical reactions involving electronically excited molecular entities which are generated thermally rather than by absorption of electromagnetic radiation. The use of this term is discouraged.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2235

dark reaction (darkness reaction)

A chemical reaction that does not require or depend on the presence of light. Contrasts with a photochemical reaction which is initiated by light absorption by one or more of the reactants.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

DAS

Acronym for decay-associated spectra.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 320

data reduction

The process of transforming the initial representation of a spectrometer output into a form which is amenable to interpretation; for example, a bar graph or a table of ion currents.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1544

dative bond

The coordination bond formed upon interaction between molecular species, one of which serves as a donor and the other as an acceptor of the electron pair to be shared in the complex formed, *e.g*, the $N \longrightarrow B$ bond in $H_3N \longrightarrow BH_3$. In spite of the analogy of dative bonds with covalent bonds, in that both types imply sharing a common electron pair between two vicinal atoms, the former are distinguished by their significant polarity, lesser strength, and greater length. The distinctive feature of dative bonds is that their minimum-energy rupture in the gas phase or in inert solvent follows the heterolytic bond cleavage path.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1933

Dauben–Salem–Turro rules

Set of rules proposed in 1975 to classify photochemical reactions based on correlation diagrams and under the assumption that all photochemical processes are controlled by the generation of primary products with characteristics of diradicals, i.e., considering the physical fact that the initial single excitation separates two electrons of a pair into two distinct orbitals. The reactions are classified according to their topicity, i.e., the total number and nature of available radical sites generated in the primary photochemical product.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 320

daughter ion

in mass spectrometry

An electrically charged product of reaction of a particular parent ion. In general such ions have a direct relationship to a particular precursor ion and indeed may relate to a unique state of the precursor ion. The reaction need not necessarily involve fragmentation. It could, for example, involve a change in the number of charges carried. Thus, all fragment ions are daughter ions, but not all daughter ions are necessarily fragment ions.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

daughter product

in radiochemistry

Any nuclide which follows a specified radionuclide in a decay chain.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517

Davydov splitting (factor-group splitting)

The splitting of bands in the electronic or vibrational spectra of crystals due to the presence of more than one (interacting) equivalent molecular entity in the unit cell.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2235

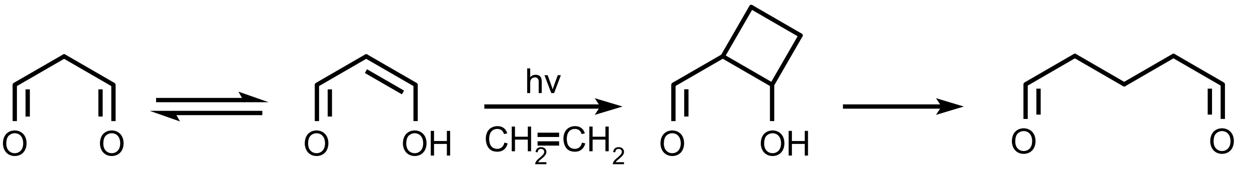
day

Non-SI unit of time, $\mathrm{d} = 86\ 400\ \mathrm{s}$. The day is not exactly defined in terms of the second since so-called leap seconds are added or subtracted from the day semiannually in order to keep the annual average occurrence of midnight at 24:00 on the clock.

Source:
Green Book, 2nd ed., p. 111
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 968

de Mayo reaction

Photochemical process leading to the formation of cyclobutanols by cycloaddition of an alkene to a 1,3-dicarbonyl-enol. The enol originates in most cases from the tautomerization of a 1,3-dicarbonyl compound. The products of the de Mayo reaction are susceptible to undergo a retro-aldol ring opening resulting in the formation of 1,5-dicarbonyl compounds.



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 322

de-electronation [obsolete]

See: oxidation (1)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1104

deactivation

Any loss of energy by an excited molecular entity.
See: emission, energy transfer, internal conversion, radiationless deactivation (decay), radiationless transition, radiative transition

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2235

dead time correction

in radioanalytical chemistry

Correction to be applied to the observed number of pulses in order to take into account the number of pulses lost during the resolving or dead time.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518

dead time

in radioanalytical chemistry

Of a radiation counter, the constant and known value imposed on the resolving time, usually in order to make the correction for resolving time losses more accurate.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517

dead time

of an analyser

The time which elapses between the moment at which a sudden change in concentration (or a new sample) is introduced and the moment at which the detector response indication reaches the measurement threshold of the analyser, a value conventionally fixed at 10% of the final change in indication.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

dead-volume [obsolete]

in chromatography

This term is used to express the extra-column volume. Strictly speaking, the term 'dead-volume' refers to volumes within the chromatographic system which are not swept by the mobile phase. On the other hand, mobile phase is flowing through most of the extra-column volumes. Due to this ambiguity the use of term 'dead-volume' is discouraged.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 833

See also:
Orange Book, p. 101

debye

Non-SI unit of electric dipole moment. It is equal to the electric dipole moment for two charges of 10^{-10} franklin separated by 1 ångström, $\mathrm{D} = 10^{-18}\ \mathrm{Fr\ cm} \approx 3.335\ 64 \times 10^{-30}\ \mathrm{C\ m}$.

Source:
Green Book, 2nd ed., p. 115

Debye–Hückel equation

The chemical potential or activity of ions cannot be determined on a purely thermodynamic basis. This is due to the fact that the effects of an ion cannot be separated from the effects of the accompanying counter-ion, or in other terms, the electrochemical potential of the ion cannot be separated into the chemical and the electrical component. Such a separation must necessarily be based on a non-thermodynamic convention. The present convention is based on the assumption that the molal activity coefficient of the chloride ion in dilute aqueous solutions ($I < 0.10\ \mathrm{mol\ kg^{-1}}$) can be estimated by means of the Debye–Hückel equation:

$$-\log_{10}\gamma_{\mathrm{B}} = \frac{z_{\mathrm{B}}{}^{2} A \sqrt{I}}{1 + å\, B \sqrt{I}}$$

where I is ionic strength, z is the charge number of the ion, $å$ is ion size parameter and A and B are temperature-dependent constants. According to the Bates–Guggenheim convention $å\, B$ is taken to be $1.5 \sqrt{\mathrm{mol\ kg^{-1}}}$ at all temperatures and for all compositions of the solutions.
See also: pH

Source:
PAC, 1984, *56*, 567 *(Physicochemical quantities and units in clinical chemistry with special emphasis on activities and activity coefficients (Recommendations 1983))* on page 569

deca

SI prefix for 10 (symbol: da).

Source:
Green Book, 2nd ed., p. 74

decadic absorbance, *A*

The negative decadic logarithm of one minus absorptance as measured on a uniform sample:

$$A = -\log_{10}(1 - \alpha)$$

Source:
PAC, 1985, *57*, 105 *(Names, symbols, definitions and units of quantities in optical spectroscopy (Recommendations 1984))* on page 116

decay chain

Synonyms: radioactive chain, radioactive series

A series of nuclides in which each member transforms into the next through nuclear decay until a stable nuclide has been formed. Synonymous with radioactive chain and radioactive series.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518

decay constant

Proportionality constant relating the activity of a radioactive substance, **A**, to the number of decaying particles **B**, N_{B}, $A = \lambda\, N_{\mathrm{B}}$. Probability of a nuclear decay within a time interval divided by that time interval. Synonymous with disintegration constant.

Source:
Green Book, 2nd ed., p. 22

See also:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 968

decay curve

A graph showing the relative amount of radioactive substance remaining after any time interval.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518

decay rate

in atmospheric chemistry

The rate at which a pollutant is removed from the atmosphere either by reaction with reactive transient species such as the HO radical, O_3, etc., by photodecomposition initiated by light absorption by the impurity, or by loss at the surface of aerosols, the earth, etc. The decay rate as applied to radioactive materials is related to the radioactive half-life ($t_{1/2}$) of the particular isotopic species **A** and its concentration $[\mathrm{A}]_t$, at the given time (t):

$$\mathrm{Rate} = \frac{[\mathrm{A}]_t \ln 2}{t_{1/2}}.$$

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

decay scheme

in radioanalytical chemistry

A graphical representation of the energy levels of the members of a decay chain showing the way along which nuclear decay occurs.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1539

decay time

in heterogenous catalysis

The time on stream during which the rate constant for the catalytic reaction, k, falls to a specified fraction of its original value, often 0.5.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 83

deci

SI prefix for 10^{-1} (symbol: d).

Source:
Green Book, 2nd ed., p. 74

decibel

Non-SI unit for expressing power levels, $\mathrm{dB} = 0.1151293\ \mathrm{Np}$.

Source:
Green Book, 2nd ed., p. 79

decomposition

The breakdown of a single phase into two or more phases. The term applies also to other chemical entities such as a normal molecule and a reaction intermediate.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 580

decontamination factor

in liquid-liquid distribution

The ratio of the proportion of contaminant to product before treatment to the proportion after treatment. It is the reciprocal of the enrichment factor.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2381

definitive method

A method of exceptional scientific status which is sufficiently accurate to stand alone in the determination of a given property for the certification of a reference material. Such a method must have a firm theoretical foundation so that systematic error is negligible relative to the intended use. Analyte masses (amounts) or concentrations must be measured directly in terms of the base units of measurements, or indirectly related through sound theoretical equations. Definitive methods, together with certified reference materials, are primary means for transferring accuracy, i.e. establishing traceability.

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1701

deflection (for a precision balance)

(In terms of divisions of the pointer scale). The other point of reversal of an ideal (undamped) swing starting at the zero point of the pointer scale. Since the points of reversal of an ideal swing are located symmetrically about the rest point, the deflection is equal to twice the rest point.

Source:
Orange Book, p. 36

deflocculation (peptization)

The reversal of coagulation or flocculation, i.e. the dispersion of aggregates to form a colloidally stable suspension or emulsion.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

degeneracy

Synonym: statistical weight

Number of states having the same energy. Symbols: g, d, W, ω, β. Also called statistical weight.

Source:
Green Book, 2nd ed., p. 39

degenerate chain branching

Sometimes chain branching is brought about by an intermediate which has a long lifetime compared with an ordinary free radical. If this intermediate can break down in different ways, only one of which leads to branching, there may be a relatively slow increase in the number of radicals, and there is said to be degenerate chain branching.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 162

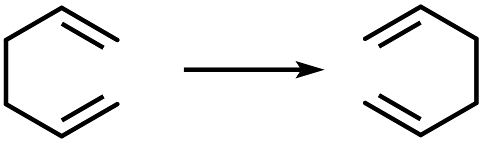
degenerate orbitals

Orbitals whose energy levels are equal in the absence of external fields. Any linear combination of the functions corresponding to a given set of degenerate orbitals serves as an equivalent representation of this set of orbitals.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1933

degenerate rearrangement

A molecular rearrangement in which the principal product is indistinguishable (in the absence of isotopic labelling) from the principal reactant. The term includes both 'degenerate intramolecular rearrangements' and reactions that involve intermolecular transfer of atoms or groups ('degenerate intermolecular rearrangements'): both are degenerate isomerizations. The occurrence of degenerate rearrangements may be detectable by isotopic labelling or by dynamic NMR techniques. For example: the [3,3]sigmatropic rearrangement of hexa-1,5-diene (Cope rearrangement):



Synonymous but less preferable terms are 'automerization', 'permutational isomerism', 'isodynamic transformation', 'topomerization'.
See also: fluxional, molecular rearrangement, valence isomer

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1104

degree Celsius

SI derived unit of Celsius temperature equal to the kelvin (symbol: °C).

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 968

degree Fahrenheit

Non-SI unit of Fahrenheit temperature, $^\circ\mathrm{F} = \frac{5}{9}\,\mathrm{K}$. The Fahrenheit temperature is related to the Celsius temperature by $\frac{\theta_\mathrm{F}}{^\circ\mathrm{F}} = \frac{9}{5}\frac{\theta}{^\circ\mathrm{C}} + 32$.

Source:
Green Book, 2nd ed., p. 113

degree

of arc

Non-SI unit of plane angle, $1\ ^\circ = \frac{\pi}{180}\ \mathrm{rad} \approx 0.017\ 453\ 29\ ...\ \mathrm{rad}$.

Source:
Green Book, 2nd ed., p. 113
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 968

degree of association

of a micelle

The number of surfactant ions in the micelle. It does not concern the location of the counterions.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

degree of crystallinity

of a polymer

The fractional amount of crystallinity in the polymer sample (w_c for mass fraction; φ_c for volume fraction).

Notes:

1. The assumption is made that the sample can be subdivided into a crystalline phase and an amorphous phase (the so-called two-phase model).
2. Both phases are assumed to have properties identical with those of their ideal states, with no influence of interfaces.
3. The degree of crystallinity may be expressed either as the mass fraction or as the volume fraction, the two quantities being related by $w_\mathrm{c} = \frac{\varphi_\mathrm{c}\,\rho_\mathrm{c}}{\rho}$ where ρ and ρ_c are the densities of the entire sample and of the crystalline fraction, respectively.
4. The degree of crystallinity can be determined by several experimental techniques; among the most commonly used are: (i) X-ray diffraction, (ii) calorimetry, (iii) density measurements, and (iv) infrared spectroscopy (IR). Imperfections in crystals are not easily distinguished from the amorphous phase. Also, the various techniques may be affected to different extents by imperfections and interfacial effects. Hence, some disagreement among the results of quantitative measurements of crystallinity by different methods is frequently encountered.

Source:
Purple Book, p. 75

degree of dissociation

Degree of reaction for a dissociation reaction.

Source:
Green Book, 2nd ed., p. 43

PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 968

degree of ionization

Degree of reaction for an ionization reaction.

Source:
Green Book, 2nd ed., p. 43

degree of polymerization

The number of monomeric units in a macromolecule or oligomer molecule, a block or a chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2291

degree of reaction, α

Extent of reaction divided by the maximum extent of reaction.

Source:
Green Book, 2nd ed., p. 43

degrees of cistacticity and transtacticity

For a regular polymer containing double bonds in the main chain of the constitutional repeating units these are the fractions of such double bonds that are in the *cis* and *trans* configurations, respectively.

Source:
Purple Book, p. 46

degrees of freedom, ν

A statistical quantity indicating the number of values which could be arbitrarily assigned within the specification of a system of observations. For simple replication, with n measurements and one estimated parameter (the mean), $\nu = n - 1$. More generally, for multivariable computations, the number of degrees of freedom equals the number of observations minus the number of fitted parameters.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 599

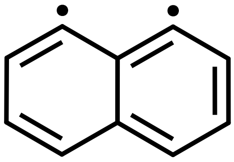
degrees of triad isotacticity, syndiotacticity, and heterotacticity

The fractions of triads in a regular vinyl polymer that are of the *mm*, *rr* and *mr* = *rm* types, respectively. In cases where triad analysis is not attainable, the diad isotacticity and diad syndiotacticity may be defined as the fractions of diads in a regular vinyl polymer that are of the *m* and *r* types, respectively. (*m* = *meso*; *r* = *racemic*).

Source:
Purple Book, p. 45

dehydroarenes

Species, usually transient, derived formally by the abstraction of a hydrogen atom from each of two ring atoms of an arene. The name for specific compounds requires the numerical prefix di-. E.g. 1,8-didehydronaphthalene or naphthalene-1,8-diyl.



1,2-Didehydroarenes are called arynes and are commonly represented with a formal triple bond.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

dehydrobenzenes

A subclass of dehydroarenes.
See: benzynes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

delayed coincidence

The occurrence of two or more events separated by a short but measurable time interval.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

delayed coke

A commonly used term for a primary carbonization product (green or raw coke) from high-boiling hydrocarbon fractions (heavy residues of petroleum or coal processing) produced by the delayed coking process.

Note:
Delayed coke has, with only a few exceptions, a better graphitizability than cokes produced by other coking processes even if the same feedstock is used. Delayed coke contains a mass fraction of volatile matter between 4 and 15 wt% which can be released during heat treatment.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 486

delayed coking process

A thermal process which increases the molecular aggregation or association in petroleum-based residues or coal tar pitches leading to extended mesophase domains. This is achieved by holding them at an elevated temperature (usually $750 - 765\ \mathrm{K}$) over a period of time (12 to $36\ \mathrm{h}$). It is performed in a coking drum and is designed to ultimately produce delayed coke The feed is rapidly pre-heated in a tubular furnace to about $760\ \mathrm{K}$.
Note:
Needle coke is the premium product of the delayed coking process. It is generally produced from highly aromatic residues from, for instance, the steam cracking of gas oil. Its appearance and preferred orientation of the graphene layers is a consequence of the evolved gaseous products percolating through the mesophase which must not have too high a viscosity. A close control of temperature, time and feedstock is essential. Lower grades, for instance isotropic cokes, are used for carbon electrodes applied, for example, in the production of aluminium.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 486

delayed fluorescence

Also contains definition of: recombination fluorescence

Three types of delayed fluorescence are known:
1. E-type delayed fluorescence: The process in which the first excited singlet state becomes populated by a thermally activated radiationless transition from the first excited triplet state. Since in this case the populations of the singlet and triplet states are in thermal equilibrium, the lifetimes of delayed fluorescence and the concomitant phosphorescence are equal.
2. P-type delayed fluorescence: The process in which the first excited singlet state is populated by interaction of two molecules in the triplet state (triplet-triplet annihilation) thus producing one molecule in the excited singlet state. In this biphotonic process the lifetime of delayed fluorescence is half the value of the concomitant phosphorescence.
3. Recombination fluorescence: The first excited singlet state becomes populated by recombination of radical ions with electrons or by recombination of radical ions of opposite charge.

See also: delayed luminescence

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 233

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2235
Orange Book, p. 185

delayed luminescence

Luminescence decaying more slowly than that expected from the rate of decay of the emitting state. The following mechanisms of luminescence provide examples:

1. triplet-triplet or singlet-singlet annihilation to form one molecular entity in its excited singlet state and another molecular entity in its electronic ground state (sometime referred to as P type),
2. thermally activated delayed fluorescence involving reversible intersystem crossing (sometimes referred to as E type), and
3. combination of oppositely charged ions or of an electron and a cation. For emission to be referred to in this case as delayed luminescence at least one of the two reaction partners must be generated in a photochemical process.

See also: delayed fluorescence

Source:
PAC, 1988, *60*, 1055 *(Glossary of terms used in photochemistry (Recommendations 1988))* on page 1065

See also:
Orange Book, p. 185

delayed neutrons

Neutrons emitted by fission products formed by nuclear decay (the observed delay is due to the preceding nuclear decay or decays).

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

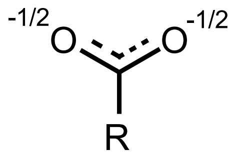
deliquescence

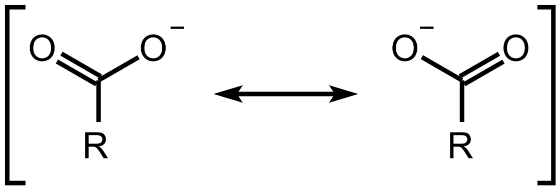
The process that occurs when the vapour pressure of the saturated aqueous solution of a substance is less than the vapour pressure of water in the ambient air. When water vapour is collected by the pure solid compound, a mixture of the solid and liquid or an aqueous solution of the compound forms until the substance is dissolved and is in equilibrium with its environment; at this time the vapour pressure of water over the aqueous solution will equal the partial pressure of water in the atmosphere in contact with it. A crystalline salt aerosol particle will deliquesce in the atmosphere when the relative humidity surpasses a characteristic value, the so-called deliquescence point.

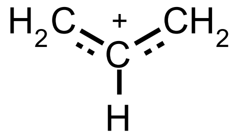
Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

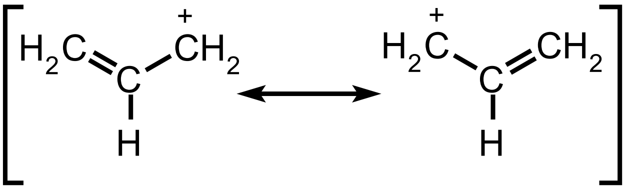
delocalization

A quantum mechanical concept most usually applied in organic chemistry to describe the π-bonding in a conjugated system. This bonding is not localized between two atoms: instead, each link has a 'fractional double bond character' or bond order. There is a corresponding 'delocalization energy', identifiable with the stabilization of the system compared with a hypothetical alternative in which formal (localized) single and double bonds are present. Some degree of delocalization is always present and can be estimated by quantum mechanical calculations. The effects are particularly evident in aromatic systems and in symmetrical molecular entities in which a lone pair of electrons or a vacant p-orbital is conjugated with a double bond (e.g. carboxylate ions, nitro compounds, enamines, the allyl cation). Delocalization in such species may be represented by partial bonds or as resonance (here symbolized by a two-headed arrow) between contributing structures.









These examples also illustrate the concomitant delocalization of charge in ionic conjugated systems. Analogously, delocalization of the spin of an unpaired electron occurs in conjugated radicals.
See also: mesomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1104

delocalization energy (DE)

The difference between the actual π-electron energy of a molecular entity and the π-electron energy of a hypothetical species with a localized form of the π-electron system. These energies are normally evaluated within Hückel molecular orbital theory.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1933

delocalization

in theoretical organic chemistry

Redistribution of the valence-shell electron density throughout a molecular entity as compared with some localized models (individual atoms in their valence states, separated bonds or fragments). Different topological modes of the electron delocalization include:

1. *ribbon delocalization* of either π- or σ-electrons (*i.e.*, electrons occupying respectively π- and σ-orbitals)
2. *surface delocalization* of σ-electrons occurring through an overlap of radially oriented σ-orbitals of a cyclic molecule, as is the case of cyclopropane; and
3. *volume delocalization* of σ-electrons through an overlap of σ-orbitals directed inside a molecular polyhedron, as is the case in tetrahedrane.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1933

demister

Apparatus made of wire mesh or glass fibre which is used to help remove acid mist as in the manufacture of sulfuric acid. Demisters are also components of wet arrestment plants.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

denaturation

of a macromolecule

The process of partial or total alteration of the native structure of a macromolecule resulting from the loss of tertiary or tertiary and secondary structure that is a consequence of the disruption of stabilizing weak bonds. Denaturation can occur when proteins and nucleic acids are subjected to elevated temperature or to extremes of pH, or to non-physiological concentrations of salt, organic solvents, urea or other chemical agents.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 151
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

denaturation

of alcohol

Addition of methanol or acetone to alcohol to make it unfit for drinking.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2036

dendrite

A crystalline morphology produced by skeletal growth, leading to a 'tree-like' appearance.

Source:
Purple Book, p. 83

denitrification

The reduction of nitrates to nitrites, dinitrogen oxide (nitrous oxide) or dinitrogen catalysed by microoganisms, e.g. facultative aerobic soil bacteria under anaerobic conditions.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 151

densification

Removal of impurities and the elimination of pores from a xerogel to give a material of as near bulk density as possible.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1822

density, ρ

Mass of a sample or body divided by its volume.

Source:
Green Book, 2nd ed., p. 12
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 968

density inversion

in solvent extraction

The interchange of the denser and less dense phases due to changes in solute concentration. Phase inversion is often used in this context but is ambiguous.
See: phase inversion

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2387

density of states, N_E, $r(E)$

1. Number of states within an energy interval divided by volume and that energy interval. Symbol: N_E.
2. Number of states within an energy interval divided by that energy interval. Symbol: $r(E)$).

Source:
Green Book, 2nd ed., p. 37
Green Book, 2nd ed., p. 39
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 162

denticity

In a coordination entity the number of donor groups from a given ligand attached to the same central atom.
See: chelation

Source:
Red Book, p. 147

denuder system (tube or assembly)

An apparatus used to separate gases and aerosols (over a given diameter) which is based upon the difference in diffusion velocity between gases and aerosol particles. Usually a tube containing a selective internal wall coating which removes the gaseous compounds at the wall.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

deodorizer

in atmospheric chemistry

Equipment for the removal of noxious gases and odours, which may consist of combustion, absorption, or adsorption units.
See: emission control equipment

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

deoxyribonucleic acids (DNA)

High molecular weight, linear polymers, composed of nucleotides containing deoxyribose and linked by phosphodiester bonds; DNA contain the genetic information of organisms. The double-stranded form consists of a double helix of two complementary chains that run in opposite directions and are held together by hydrogen bonds between pairs of the complementary nucleotides and Hoogsteen (stacking) forces.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 151

depolarization of scattered light

The phenomenon, due primarily to the anisotropy of the polarizability of the scattering medium, resulting from the fact that the electric vectors of the incident and scattered beams are not coplanar and that, therefore, light scattered from a vertically (horizontally) polarized incident beam contains a horizontal (vertical) component.

Source:
Purple Book, p. 67

depolarizer [obsolete]

Synonym for electroactive substance (preferred term).

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1500
Orange Book, p. 58

depolymerization

Also contains definition of: unzipping

The process of converting a polymer into a monomer or a mixture of monomers.
Note:
Unzipping is depolymerization occurring by a sequence of reactions, progressing along a macromolecule and yielding products, usually monomer molecules at each reaction step, from which macromolecules similar to the original can be regenerated.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2309

deposition

in atmospheric chemistry

Deposition is normally considered to be one of two types: dry deposition is the process by which aerosols and gases in the air are deposited on the surface of the earth (soil, water, rock, plants, etc.); this is termed 'dry' deposition even when the receptor surface is moist. Wet deposition is that process which involves the transport of chemicals to the surface of the earth by water droplets or snow crystals which scavenge pollutants as they form and fall through the atmosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

deposition velocity

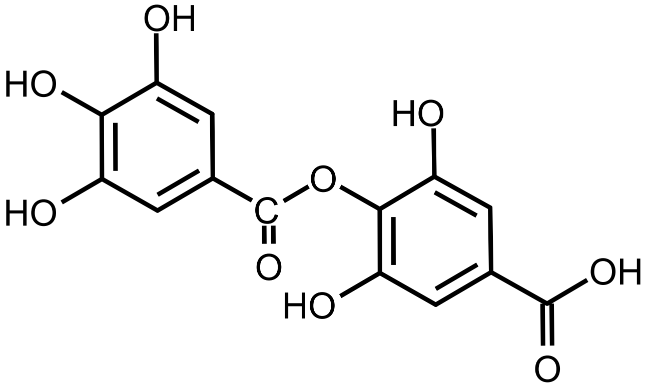
in atmospheric chemistry

The ratio of flux density (often given in units of $g\ cm^{-2}\ s^{-1}$) of a substance at a sink surface to its concentration in the atmosphere (corresponding units of $g\ cm^{-3}$). While the units of this ratio are clearly those of velocity (in this case $cm\ s^{-1}$), the ratio is not a flow velocity in the normal sense of the word.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

depsides

Intermolecular esters formed from two or more molecules of the same or different phenolic benzoic acids. Depending on the number of the component units, di-, tri-, etc. depsides may result, e.g. 4-*O*-galloylgallic acid:

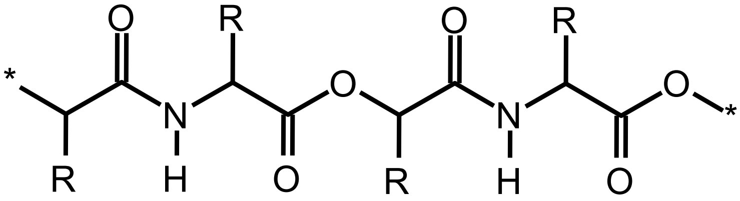


Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

depsipeptides

Also contains definition of: cyclodepsipeptides

Natural or synthetic compounds having sequences of amino and hydroxy carboxylic acid residues (usually α-amino and α-hydroxy acids), commonly but not necessarily regularly alternating. In cyclodepsipeptides, the residues are connected in a ring.



See: carboxylic acids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

See also:
PAC, 1984, *56*, 595 *(Nomenclature and symbolism for amino acids and peptides (Recommendations 1983))* on page 617

depth of penetration

of light

The inverse of the absorption coefficient. If the decadic absorption coefficient, a, is used, the depth of penetration ($\frac{1}{a}$) is the distance at which the radiant power, P_{λ}, decreases to one tenth of its incident value, P_{λ}^{0}. If the Naperian absorption coefficient, α, is used, the depth of penetration ($\frac{1}{\alpha} = \beta$ in this case) is the distance at which the radiant power decreases to $\frac{1}{\mathrm{e}}$ of its incident value.
See: absorbance, attenuance

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2235

depth profile

Dependence of concentration on depth perpendicular to the surface in a solid sample. It can be obtained by a simultaneous or sequential process of erosion and surface analysis or by measurement of the energy loss of primary backscattered particles produced by nuclear reactions.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

depth resolution

The distance between the 84 and 16 per cent levels of the depth profile of an element in a perfect sandwich sample with an infinitesimally small overlap of the components. These limits correspond to the 2σ-value of the Gaussian distribution of the signal at the interface.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

derivative potentiometric titration

A titration that involves measuring, recording, or computing the first derivative of the potential of a single indicator electrode with respect to the volume or otherwise added amount of reagent.

Source:
Orange Book, p. 65

derivative spectroscopy

The first (second, ...) derivative absorption spectrum of a molecule is defined as the first (second, ...) derivative, $\frac{\mathrm{d}A(\tilde{\nu})}{\mathrm{d}\tilde{\nu}}$ [$\frac{\mathrm{d}^2A(\tilde{\nu})}{\mathrm{d}\tilde{\nu}^2}$, ...] of the absorbance A as a function of wavenumber, $\tilde{\nu}$. Wavelengths may be used in place of wavenumbers but the shape of the derivative spectra will be slightly different. When derivative spectra are obtained at low temperature, they are called first (second, ...) derivative low temperature absorption spectra (specifying the solvent, temperature and solute concentration).

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1455

derived coherent unit

A unit constructed exclusively from base units, e.g. $\mathrm{mol\ kg^{-1}}$, $\mathrm{kg\ m^{-3}}$.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2461

derived kind of quantity

A kind of quantity characterized by an equation between base kinds of quantities, e.g. $\text{mass concentration} = \text{mass}\ (\text{length})^{-3}$.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2460

derived non-coherent unit

A unit constructed from base units and numerical factors, which may be named and symbolized, e.g. mg, $\mathrm{mol\ l^{-1}}$.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2461

derived quantity

Quantity defined, in a system of quantities, as a function of base quantities of that system.
See: quantity, base quantity

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 969

derived unit

of measurement

Unit of measurement of a derived quantity in a given system of quantities. Derived units are expressed algebraically in terms of base units by means of the mathematical symbols of multiplication and division.
See: unit *of measurement*, derived quantity

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 969

descending elution/development

in planar chromatography

A mode of operation in which the mobile phase is supplied to the upper edge of the paper or plate and the downward movement is governed mainly by gravity.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 829

desiccant

1. Drying agent.
2. In agriculture, a substance used for drying up plants and facilitating their mechanical harvesting.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2037

desolvation

in flame spectroscopy

The process of evaporation of the solvent from an aerosol of fine droplets (the droplets being the result of nebulizing a solution). Desolvation converts the aerosol into a dry aerosol consisting of a suspension of solid or molten particles of the solute.

Source:
Orange Book, p. 165

desorption

The converse of adsorption, i.e. the decrease in the amount of adsorbed substance.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 584

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

desorption (by displacement)

The process in which expulsion of a previously adsorbed component from the interfacial layer is effected by subsequent stronger adsorption of another component.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 585

desulfurization

The process by which sulfur is removed from a material such as coal or oil. It may involve one of many techniques including elutriation, froth flotation, laundering, magnetic separation, chemical treatment, etc.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

desymmetrization

The modification of an object which results in the loss of one or more symmetry elements, such as those which preclude chirality (mirror plane, centre of inversion, rotation-reflection axis), as in the conversion of a prochiral molecular entity into a chiral one.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205

desymmetrization step

The removal of the smallest possible number of symmetry elements from a molecule with or without the restriction to pointwise substitution.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205

detachment

The reverse of an attachment.
See also: electron attachment

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1105

detailed balancing (principle of)

When equilibrium is reached in a reaction system (containing an arbitrary number of components and reaction paths), as many atoms, in their respective molecular entities will pass forward, as well as backwards, along each individual path in a given finite time interval. Accordingly, the reaction path in the reverse direction must in every detail be the reverse of the reaction path in the forward direction (provided always that the system is at equilibrium). The principle of detailed balancing is a consequence for macroscopic systems of the principle of microscopic reversibility.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1105

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 162

detection efficiency

in nuclear analytical chemistry

The ratio between the number of particles or photons detected and the number of similar particles or photons emitted by the radiation source.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1539

detection limit

See: relative detection limit

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

detection limit

in analysis

The minimum single result which, with a stated probability, can be distinguished from a suitable blank value. The limit defines the point at which the analysis becomes possible and this may be different from the lower limit of the determinable analytical range.
See also: limit of detection, relative detection limit

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663

See also:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1553

detergent

A surfactant (or a mixture containing one or more surfactants) having cleaning properties in dilute solutions (soaps are surfactants and detergents).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

detoxification

1. Process, or processes, of chemical modification which make a toxic molecule less toxic.
2. Treatment of patients suffering from poisoning in such a way as to promote physiological processes which reduce the probability or severity of harmful effects.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2038

deuteriation

A term used to represent replacement of protium by deuterium. The use of the word deuteration is also acceptable.

Source:
PAC, 1988, *60*, 1115 *(Names for hydrogen atoms, ions, and groups, and for reactions involving them (Recommendations 1988))* on page 1115
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1556

deuterium

Also contains definitions of: deuteride, deuterio

A specific name for the atom ^{2}H. The cation $^{2}H^{+}$ is a deuteron the species $^{2}H^{-}$ is a deuteride anion and ^{2}H is the deuterio group.

Source:
PAC, 1988, *60*, 1115 *(Names for hydrogen atoms, ions, and groups, and for reactions involving them (Recommendations 1988))* on page 1116

deuteron

Nucleus of the ^{2}H (deuterium) atom.

Source:
Green Book, 2nd ed., p. 93
PAC, 1988, *60*, 1115 *(Names for hydrogen atoms, ions, and groups, and for reactions involving them (Recommendations 1988))* on page 1116

deviation, *d*

The difference between an observed value and the arithmetic mean of the set to which it belongs. It can be calculated by the formula:

$$d_i = x_i - \bar{x}$$

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 599
Orange Book, p. 4

See also:
VIM

devolatilizer

Material added to a sample to decrease its volatilization or that of some component of it.

Source:
Orange Book, p. 159

dew point hygrometer (cooled surface condensation)

Instrument in which the sample is passed over a cooled surface. The temperature at which dew forms on the cooled surface is a function of the water content of the gas passing over the surface.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

dew point

in atmospheric chemistry

That temperature at which water vapour present in the atmosphere is just sufficient to saturate it. When air is cooled below the dew point, the excess of water vapour appears as tiny droplets or crystals of ice depending on the temperature of the air mass. This term is also applicable to acid gases as in the problem of acid corrosion and acid smut formation.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

Dexter (electron exchange) excitation transfer

Excitation transfer occurring as a result of an electron exchange mechanism. It requires an overlap of the wavefunctions of the energy donor and the energy acceptor. It is the dominant mechanism in triplet-triplet energy transfer. The transfer rate constant, k_{ET}, is given by:

$$k_{\mathrm{ET}} \propto \frac{h}{2\,\pi} P^2 J \, \mathrm{e}^{\frac{-2\,r}{L}}$$

where r is the distance between donor (D) and acceptor (A), L and P are constants not easily related to experimentally determinable quantities, and J is the spectral overlap integral. For this mechanism the spin conservation rules are obeyed.
See also: radiative energy transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2235

dextrans

Branched poly-α-D-glucosides of microbial origin having glycosidic bonds predominantly C-1 → C-6.
See: glycosides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

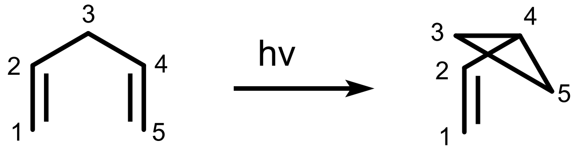
dextrins

Poly-α-D-glucosides of intermediate chain length derived from starch components (amylopectins) by the action of amylases (starch hydrolysing enzymes).
See also: cyclodextrins, dextrans

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

di-π-methane rearrangement

Photochemical reaction of a molecular entity comprising two π-systems, separated by a saturated carbon atom (a 1,4-diene or an allyl-substituted aromatic analogue), to form an ene- (or aryl-) substituted cyclopropane.
Note:
The rearrangement formally amounts to a 1,2 shift of one ene group (in the diene) or the aryl group (in the allyl-aromatic analogue) and 'bond formation' between the lateral carbons of the non-migrating moiety.

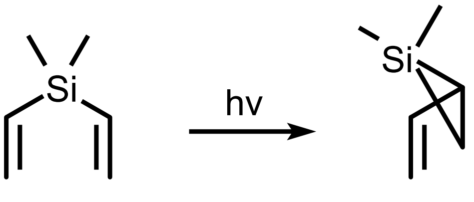


See also: aza-di-π-methane rearrangement, di-π-silane rearrangement, oxa-di-π-methane rearrangement

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 325

di-π-silane rearrangement

Silicon version of the di-π-methane rearrangement with a Si atom at position 3 of the basic 1,4-diene chromophore.



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 326

diabatic coupling

Energy coupling between two potential-energy surfaces is sometimes known as diabatic coupling.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 163

diabatic electron transfer

Electron transfer process in which the reacting system has to cross over between different electronic surfaces in passing from reactants to products. For diabatic electron transfer the electronic transmission factor is $\ll 1$ (see Marcus equation). The term non-adiabatic electron transfer has also been used and is in fact more widespread, but should be discouraged because it contains a double negation.
See also: adiabatic electron transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2236

diabatic photoreaction

Within the Born–Oppenheimer approximation, a reaction beginning on one excited state 'potential-energy surface' and ending, as a result of radiationless transition, on another surface, usually that of the ground state. Also called non-adiabatic.
See also: adiabatic photoreaction

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2235

diacylamines

Compounds having two acyl groups substituted on ammonia or a primary amine acyl-NR-acyl. They are also known as secondary amides and, especially the cyclic examples derived from diacids, as imides, e.g. $[RC(=O)]_2NR$, $RS(=O)_2NHC(=O)R$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

diagram level

in X-ray spectroscopy

A level described by the removal of one electron from the configuration of the neutral ground state. These levels form a spectrum similar to that of a one-electron or hydrogen-like atom but, being single-valency levels, have the energy scale reversed relative to that of single-electron levels. Diagram levels may be divided into valence levels and core levels according to the nature of the electron vacancy. Diagram levels with orbital angular momentum different from zero occur in pairs and form spin doublets.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 738

diagram line

in X-ray spectroscopy

See: characteristic X-ray emission, X-ray satellite

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 737

dialysate [obsolete]

After (complete or incomplete) dialysis two solutions are obtained. The one free from colloidal material is called dialysate; the other one, containing the colloidal particles may be called retentate, dialysis residue, or simply residue, but should not be called dialysate.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

dialysis

The process of separating a colloidal sol from a colloid-free solution by a membrane permeable to all components of the system except the colloidal ones, and allowing the exchange of the components of small molar mass to proceed for a certain time.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

dialysis residue

See: dialysate

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

diamagnetic

Substances having a negative magnetic susceptibility are diamagnetic. They are repelled out of a magnetic field.
See also: paramagnetic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1105

diamidides

Analogues of acyclic carboxylic acid anhydrides in which =O has been replaced by =NR and –O– by –NR–: RC(=NR)NRC(=NR)R, *N*-imidoyl amidines. The name 1,3,5-triazapentadienes is sometimes applied as a class name to diamidides.
See: imidines

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

diamond

An allotropic form of the element carbon with cubic structure (space group $O_h^7 - Fd3m$) which is thermodynamically stable at pressures above $6\ \mathrm{GPa}$ at room temperature and metastable at atmospheric pressure. At low pressures diamond converts rapidly to graphite at temperatures above $1900\ \mathrm{K}$ in an inert atmosphere. The chemical bonding between the carbon atoms is covalent with sp^3 hybridization.
Note:
There is also a hexagonal diamond-like structure of the element carbon (lonsdaleite).

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 487

diamond by CVD

Synonyms: CVD diamond, low-pressure diamond

Diamond by CVD (chemical vapour deposition) is formed as crystals or as films from various gaseous hydrocarbons or other organic molecules in the presence of activated, atomic hydrogen. It consists of sp^3-hybridized carbon atoms with the three-dimensional crystalline structure of the diamond lattice.
Note:
'CVD diamond' or 'low-pressure diamond' are synonyms of the term diamond by CVD. Diamond by CVD can be prepared in a variety of ways. Deposition parameters are: total (low) pressure, partial hydrogen pressure, precursor molecules in the gas phase, temperature for activation of the hydrogen and that of the surface of the underlying substrate. The energy supply for the hydrogen activation

may be, for instance: heat, radio frequency, microwave excitation (plasma deposition) or accelerated ions (e.g. Ar^+ ions). CVD diamond has also been obtained at atmospheric pressure from oxyacetylene torches and by other flame-based methods. Often CVD carbon films consist of a mixture of sp^2- and sp^3-hybridized carbon atoms and do not have the three-dimensional structure of the diamond lattice. In this case they should be called hard amorphous carbon or diamond-like carbon films.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 487

diamond-like carbon films

Diamond-like carbon (DLC) films are hard, amorphous films with a significant fraction of sp^3-hybridized carbon atoms and which can contain a significant amount of hydrogen. Depending on the deposition conditions, these films can be fully amorphous or contain diamond crystallites. These materials are not called diamond unless a full three-dimensional crystalline lattice of diamond is proven.
Note:
Diamond-like films without hydrogen can be prepared by carbon ion beam deposition, ion-assisted sputtering from graphite or by laser ablation of graphite. Diamond-like carbon films containing significant contents of hydrogen are prepared by chemical vapour deposition. The hydrogen content is usually over 25 atomic %. The deposition parameters are (low) total pressure, hydrogen partial pressure, precursor molecules and plasma ionization. The plasma activation can be radio frequency, microwave or Ar^+ ions. High ionization favours amorphous films while high atomic hydrogen contents favour diamond crystallite formation. Because of the confusion about structure engendered by the term diamond-like carbon films, the term hard amorphous carbon films has been suggested as a synonym.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 487

dianions

Molecular entities bearing two negative charges, which may be located on a single atom or on different atoms or may be delocalized.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

diastereoisomer (diastereoisomeric) excess

Also contains definition of: percent diastereoisomer excess

This is defined by analogy with enantiomer excess, as $D_1 - D_2$ [and the percent diastereoisomer excess as $100\,(D_1 - D_2)$], where the mole fractions of two diastereoisomers in a mixture or the fractional yields of two diastereoisomers formed in a reaction are D_1 and D_2 ($D_1 + D_2 = 1$) The term is not applicable if more than two diastereoisomers are present. Frequently this term is abbreviated to d.e.
See: stereoselectivity, diastereoisomerism

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205

diastereoisomeric units

in a polymer

Two non-superposable configurational units that correspond to the same constitutional unit are considered to be diastereomeric if they are not mirror images.

Source:
Purple Book, p. 27

diastereoisomerism

Also contains definitions of: diastereoisomers, diastereomers

Stereoisomerism other than enantiomerism. Diastereoisomers (or diastereomers) are stereoisomers not related as mirror images. Diastereoisomers are characterized by differences in physical properties, and by some differences in chemical behaviour towards achiral as well as chiral reagents.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1105

diastereoisomerization

The interconversion of diastereoisomers.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2205

diastereomeric ratio

This is defined by analogy with enantiomeric ratio as the ratio of the percentage of one diastereoisomer in a mixture to that of the other.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2206

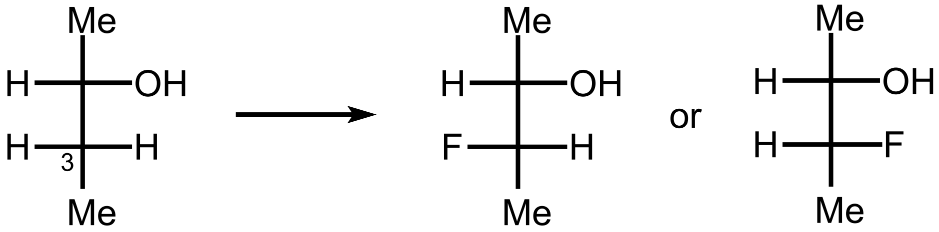
diastereomorphism

The relationship between objects (or models) analogous to that between diastereoisomeric molecular entities.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2206

diastereotopic

Constitutionally equivalent atoms or groups of a molecule which are not symmetry related. Replacement of one of two diastereotopic atoms or groups results in the formation of one of a pair of diastereoisomers. In the example below the two hydrogen atoms of the methylene group C-3 are diastereotopic.



See also: prochirality, enantiotopic, heterotopic

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2206

diazanylidenes

An alternative term for isodiazenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1331

diazenyl radicals

Radicals of structure $RN{=}N^{\cdot}$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

diazo compounds

Compounds having the divalent diazo group, $=N^{+}{=}N^{-}$, attached to a carbon atom, e.g. $CH_2{=}N_2$ diazomethane.
See also: dipolar compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

diazoamino compounds

Compounds having the structure $RN{=}N{-}NR_2$ (not all R = H, and one R commonly aryl). In systematic nomenclature, diazoamino prefixed to the name of RH names the compound RN=NNHR' (R = R'), e.g. PhN=N–NPhMe *N*-methyldiazoaminobenzene.
See also: triazenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

diazoates

Also contains definition of: diazotates

Salts $RN{=}NO^{-}M^{+}$ (R commonly aryl) of the compounds RN=NOH , (hydrocarbon)diazohydroxides, e.g. $PhN{=}NO^{-}K^{+}$ potassium benzenediazoate. In the IUPAC 'Blue Book' these compounds are named as hydrocarbyldiazenolates and hydrocarbyldiazenols, respectively. E.g. PhN=NOH phenyldiazenol. $RN{=}NO^{-}M^{+}$ are also known by the non-IUPAC name diazotates.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

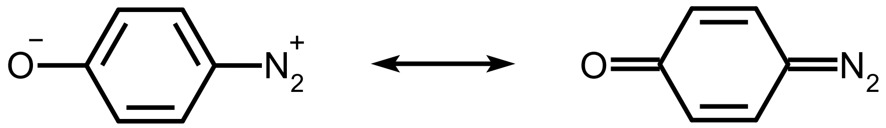
diazonium salts

Compounds of structure $RN_2{}^{+}Y^{-}$, in which R is generally but not necessarily aryl, and the cations of which are usually formulated as $RN^{+}{\equiv}N$, E.g. $PhN^{+}{\equiv}N$ benzenediazonium chloride. They may also be named, from the canonical form $RN{=}N^{+}$, hydrocarbyldiazenylium salts.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

diazooxides

Diazocyclohexadienones, which may also be considered as dipolar diazonio phenoxides, obtained by diazotizing aromatic primary amines having a hydroxy group in an *ortho* or *para* position. Also known as diazophenols.



See also: diazo compounds, phenoxides, quinone diazides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

dicarbenium ions

Species carrying two positive charges, formally located on tervalent carbon atoms, e.g. $^+CH_2–^+CH_2$ ethane-1,2-diyl dication, $^+CH_2CH_2–^+CH_2$ propane-1,3-bis(ylium).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

dichotomous sampler

Device for dividing a polydispersed aerosol particle population into two size fractions during sampling. The fractionation is based on the momentum differences of the particles which allow the larger particles to pass through a zone of stagnant gas.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2212

dichroic filter

Note:
The name dichroic arises from the fact that the filter appears one colour under illumination with transmitted light and another with reflected light.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 323

dichroic mirror

A mirror used to reflect light selectively according to its wavelength.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 323

dichroism

Dependence of absorbance of a sample on the type of polarization of the measuring beam. This polarization may be linear, corresponding to linear dichroism (LD) in which the difference in absorption for two perpendicularly linearly polarized beams is measured, $\Delta A_l = A_Z - A_Y$, or circular dichroism (CD) in which the difference in absorption for left minus right circularly polarized beams is measured, $\Delta A_C = A_L - A_R$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 324

dielectric constant **[obsolete]**

See: relative permittivity

Source:
Green Book, 2nd ed., p. 14

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1105

dielectric polarization, *P*

The difference between the electric displacement vector and the product of the electric field strength with the permittivity of vacuum, $\boldsymbol{P} = \boldsymbol{D} - \varepsilon_0 \boldsymbol{E}$.

Source:
Green Book, 2nd ed., p. 14

dienes

Compounds that contain two fixed double bonds (usually assumed to be between carbon atoms). Dienes in which the two double-bond units are linked by one single bond are termed conjugated, e.g. $CH_2{=}CH{-}CH{=}CH_2$ buta-1,3-diene. Dienes in which the double bonds are adjacent are called cumulative, e.g. $CH_3{-}CH{=}C{=}CH_2$ buta-1,2-diene. Those in which one or more of the unsaturated carbon atoms is replaced by a heteroatom may be called heterodienes.
See: alkenes, olefins, diols, allenes, cumulenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

dienophile

The olefin component of a Diels–Alder reaction.
See: cycloaddition

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1105

difference absorption spectroscopy

A highly concentrated analyte in an analytical sample can be determined with better precision by replacing the blank (reference) cell by one containing a solution of the analyte or other absorber of known concentration; this is known as difference absorption spectroscopy. Difference spectra can also be obtained by computer or other subtraction methods.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1455

differential capacitance

Differential capacitance (per unit area of interphase or electrode; SI unit $\mathrm{F\ m^{-2}}$) is given by

$$C = \left(\frac{\partial Q}{\partial E}\right)_{T,p,\mu_i,\ldots}$$

where E is the potential of the electrode with respect to a reference electrode, μ_i is a set of chemical potentials which are held constant, T is the thermodynamic temperature, Q is the electric charge (per unit area of interphase or electrode), and p is the pressure.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 509
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1261

differential detector

in chromatography

A device which measures the instantaneous difference in the composition of the column effluent.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 849
Orange Book, p. 99

differential diffusion coefficient

Also contains definition of: limiting differential diffusion coefficient

Defined by

$$D_i = \frac{-\boldsymbol{J}_i}{\nabla c_i}$$

where $\boldsymbol{J}_i$ is the amount of species i flowing through unit area in unit time and ∇c_i is the concentration gradient of species i. Different diffusion coefficients may be defined depending on the choice of the frame of reference used for $\boldsymbol{J}_i$ and ∇c_i. For systems with more than two components, the flow of any component and hence its diffusion coefficient depends on the concentration distribution of all components. The limiting differential diffusion coefficient is the value of D_i extrapolated to zero concentration of the diffusing species:

$$[D_i] = \lim_{c_i \to 0} D_i$$

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 617

differential molar energy of adsorption

Also contains definitions of: differential molar interfacial energy, differential molar surface excess energy

When the addition of a differential amount $\mathrm{d}n_i^\sigma$ or $\mathrm{d}n_i^\mathrm{s}$ is effected at constant gas volume, the differential molar energy of adsorption of component i, $\Delta_a U_i^\sigma$ or $\Delta_a U_i^\mathrm{s}$, is defined as:

$$\Delta_a U_i^\sigma = U_i^\sigma - U_i^\mathrm{g}$$

or

$$\Delta_a U_i^s = U_i^\mathrm{s} - U_i^\mathrm{g}$$

where the differential molar surface excess energy, U_i^σ, is given by

$$U_i^\sigma = \left(\frac{\partial U^\sigma}{\partial n_i^\mathrm{s}}\right)_{T,m,n_j^\sigma} = \left(\frac{\partial U}{\partial n_i^\sigma}\right)_{T,m,V^\mathrm{g},p_i,n_j^\sigma}$$

and the differential molar interfacial energy, U_i^s, by

$$U_i^{\mathrm{s}} = \left(\frac{\partial U}{\partial n_i^{\mathrm{s}}}\right)_{T,m,V^{\mathrm{g}},p_i,n_j^{\sigma}} = \left(\frac{\partial U}{\partial n_i^{\mathrm{s}}}\right)_{T,m,V^{\mathrm{g}},V^{\mathrm{s}},p_i,n_j^{\mathrm{s}}}$$

U_i^{g} is the differential molar energy of component i in the gas phase, i.e.

$$\left(\frac{\partial U}{\partial n_i^{\mathrm{g}}}\right)_{T,V,n_i^{\mathrm{g}}}$$

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 603

differential scanning calorimetry (DSC)

A technique in which the difference in energy inputs into a substance (and/or its reaction product(s)) and a reference material is measured as a function of temperature whilst the substance and reference material are subjected to a controlled temperature programme.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1739
Orange Book, p. 44

differential thermal analysis (DTA)

A technique in which the temperature difference between a substance and a reference material is measured as a function of temperature, while the substance and reference material are subjected to a controlled temperature program.

Source:
Orange Book, p. 42

differential viscosity

The derivative η_Δ of stress with respect to the rate of shear at a given shear rate.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

diffraction

A modification which light (or electron, neutron beams, etc.) undergoes in passing by the edges of opaque bodies or through narrow slits or in being reflected from ruled surfaces (or crystalline materials). The light waves, owing to their wave-like nature appear to be deflected and produce fringes of parallel light and dark bands corresponding to regions of constructive reinforcement or destructive interference, respectively, of the waves.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

diffraction analysis

The application of diffraction techniques (X-rays, electrons, neutrons) which are sometimes used to identify the presence of certain solid aerosols and dust particles through the characteristic diffraction patterns which result from each unique crystal structure.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

diffuse layer
Also contains definition of: Gouy layer *in electrochemistry*

in electrochemistry

The region in which non-specifically adsorbed ions are accumulated and distributed by the contrasting action of the electric field and thermal motion. Counter and co-ions in immediate contact with the surface are said to be located in the Stern layer. Ions farther away from the surface form the diffuse layer or Gouy layer.
See also: interfacial double-layer

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1261
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 618

diffused junction semiconductor detector

A semiconductor detector in which the p–n or n–p junction is produced by diffusion of donor or acceptor impurities.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1540

diffuser

A porous plate or tube, commonly made of carborundum, alundum or silica sand, through which air is forced and divided into minute bubbles for diffusion in liquids.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

diffusion

The spreading or scattering of a gaseous or liquid material. Eddy diffusion in the atmosphere is the process of transport of gases due to turbulent mixing in the presence of a composition gradient. Molecular diffusion is the net transport of molecules which results from their molecular motions alone in the absence of turbulent mixing; it occurs when the concentration gradient of a particular gas in a mixture differs from its equilibrium value. Eddy diffusion is the most important mixing process in the lower atmosphere, while molecular diffusion becomes significant at the lower pressures of the upper atmosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

diffusion battery

An aerosol sizing instrument for particles with diameters below $0.2\ \mu\mathrm{m}$. The fractionation is based on different diffusivities of the small particles and their deposition on the walls of the long parallel or circular channels, formed by equally spaced plates, bundles of small bore parallel tubes or sets of stainless wire screens.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

diffusion coefficient, D

Proportionality constant D, relating the flux of amount of entities **B** to their concentration gradient $\boldsymbol{J}_n = -D\, \nabla c_{\mathrm{B}}$.

Source:
Green Book, 2nd ed., p. 65

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 969

diffusion control

See: microscopic diffusion control

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 163

diffusion current constant

in polarography

The empirical quantity defined by the equation

$$i = \frac{i_{\mathrm{d},l}}{c_{\mathrm{B}}\, m^{\frac{2}{3}}\, t_1^{\frac{1}{6}}}$$

where $i_{\mathrm{d},l}$ = limiting diffusion current, c_{B} = bulk concentration of the substance **B** whose reduction or oxidation is responsible for the wave in question, m = average rate of (mass) flow of mercury (or other liquid metal) and t_1 = drop time.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1500

diffusion current (or diffusion-controlled current)

A faradaic current whose magnitude is controlled by the rate at which a reactant in an electrochemical process diffuses toward an electrode-solution interface (and, sometimes, by the rate at which a product diffuses away from that interface). For the reaction mechanism

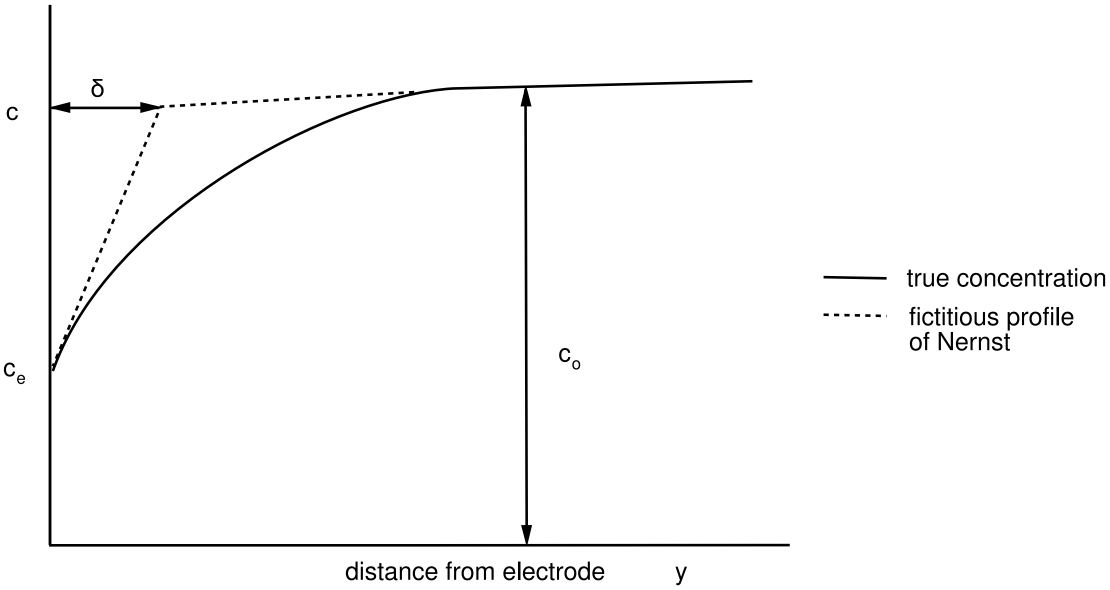
$$\mathrm{C} \underset{k_-}{\overset{k}{\rightleftharpoons}} \mathrm{B} \xrightarrow{+\,n\,e} \mathrm{B'}$$

there are two common situations in which a diffusion current can be observed. In one, the rate of formation of B from electroinactive C is small and the current is governed by the rate of diffusion of B toward the electrode surface. In the other, C predominates at equilibrium in the bulk of the solution, but its transformation into B is fast; C diffuses to the vicinity of the electrode surface and is there rapidly converted into B, which is reduced.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1495

diffusion layer (concentration boundary layer)

The region in the vicinity of an electrode where the concentrations are different from their value in the bulk solution. The definition of the thickness of the diffusion layer is arbitrary because the concentration approaches asymptotically the value c_0 in the bulk solution (see diagram).



See also: Nernst's diffusion layer

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1837

diffusion layer thickness

Defined by the equation:

$$\delta = \frac{D}{k_{\mathrm{d}}} = \frac{n\,F\,D\,c\,A}{l_i}$$

where D is the diffusion coefficient, k_{d} is the heterogeneous diffusion rate constant, F is the Faraday constant, c is the concentration, A is the geometric area of the electrode, l_i is the limiting current and n is the charge number of the cell reaction.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 513

diffusion potential

For an ideal dilute solution, $\Delta\Phi_{\mathrm{d}}$ is the integral of $\nabla\,\Phi$ (given by the following equation) across the boundary between two regions of different concentrations.

$$\nabla \Phi = \frac{R\,T \sum D_i\, z_i\, \nabla c_i}{F \sum s_i^2\, D_i\, c_i}$$

where D_i is the diffusion coefficient of species i, z_i is the charge number of species i, c_i is the concentration of species i, R is the gas constant, T is the thermodynamic temperature, and F is the Faraday constant.

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1838

diffusion-controlled rate

See: encounter-controlled rate, macroscopic diffusion control, microscopic diffusion control

Source:
PAC, 1983, *55*, 1281 *(Glossary of terms used in physical organic chemistry)* on page 1308

diffusional transition

A transition that requires the rearrangement of atoms, ions or molecules in a manner that cannot be accomplished by a cooperative atomic displacement; it may require the movement of atoms, ions or molecules over distances significantly larger than a unit cell. Example: The transition of graphite (hexagonal sheets of three-coordinated carbon atoms) to diamond (infinite three-dimensional framework of four-coordinated carbon atoms) at high temperature and pressure.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 581

diffusionless transition

A transition that does not involve long-range diffusion of atomic species over distances significantly greater than a typical interatomic distance.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 581

dihedral angle

The angle between two intersecting planes on a third plane normal to the intersection of the two planes.
See: torsion angle

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2206

diisotactic polymer

An isotactic polymer that contains two chiral or prochiral atoms with defined stereochemistry in the main chain of the configurational base unit.

Source:
Purple Book, p. 32

dilatancy

An increase in volume of the system which usually accompanies shear thickening. This term has formerly been used for the phenomenon of shear thickening.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

dilational (dilatational) transition

A transition in which the crystal structure is dilated (or compressed) along one (or more) crystallographic direction(s) while the symmetry about that direction is retained. Examples:

1. The transition of a CsCl-type structure to a rock salt structure in which dilation occurs along the three-fold axis.
2. The transition at T_D in quenched NiS in which volume expansion occurs without change of symmetry on going from a metallic state ($T > T_\mathrm{D}$) to a semiconducting state ($T < T_\mathrm{D}$).

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 581

diluent gas

A gas of known quality introduced for analytical purposes so that it quantitatively lowers the concentration of the components of a gaseous sample; this may also be the complementary gas.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

diluent
Also contains definition of: cosolvent

in solvent extraction

The liquid or homogeneous mixture of liquids in which extractant(s) and possible modifier(s) may be dissolved to form the solvent phase.
Notes:

1. The term carrier, which implies an inert diluent is not recommended.
2. Although the diluent may well be a single liquid or even the major portion of the extracting phase, the term solvent should not be used in this sense as it has a much wider meaning in the context of liquid-liquid extraction, although the term cosolvent may be used in certain circumstances.
3. The diluent by itself does not extract the main (extractable) solute appreciably.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2380

dilute solution

Solution in which the sum of amount fractions of all the solutes is small compared to 1.

Source:
Physical Chemistry Division, unpublished
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 535

See also:
Purple Book, p. 57

diluter

A device used to add a measured volume or amount of the sample to a measured volume of a diluent.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

dilution rate, *D*

in biotechnology

The ratio of the ingoing volume flow rate ($\frac{\mathrm{d}V}{\mathrm{d}t}$) and the culture volume (V). In continuous fermentation, a measure of a rate at which the existing medium is replaced with fresh medium, D is the reciprocal of the hydraulic retention time (HRT).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 152

dimension

of a quantity

Product of powers of the base dimensions (the dimensions attributed to the base quantities of a system) which parallels the expression of the quantity in terms of the base quantities. When all the exponents of the base dimensions are zero the quantity has the dimension one and is often called dimensionless.

Source:
Physical Chemistry Division, unpublished
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 969

dimensionless quantities

Quantities of dimension one, or numerical quantities, are numbers which may be integers (or exceptionally half-integers) when obtained by counting (e.g. number of molecules, quantum numbers, ...), rational numbers such as ratios, factors and fractions when obtained as ratios of two quantities of the same kind or real numbers when obtained by taking logarithms (e.g. absorbance, power levels, ...).

Source:
Green Book, 2nd ed., p. 77
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 969

dimeric ion

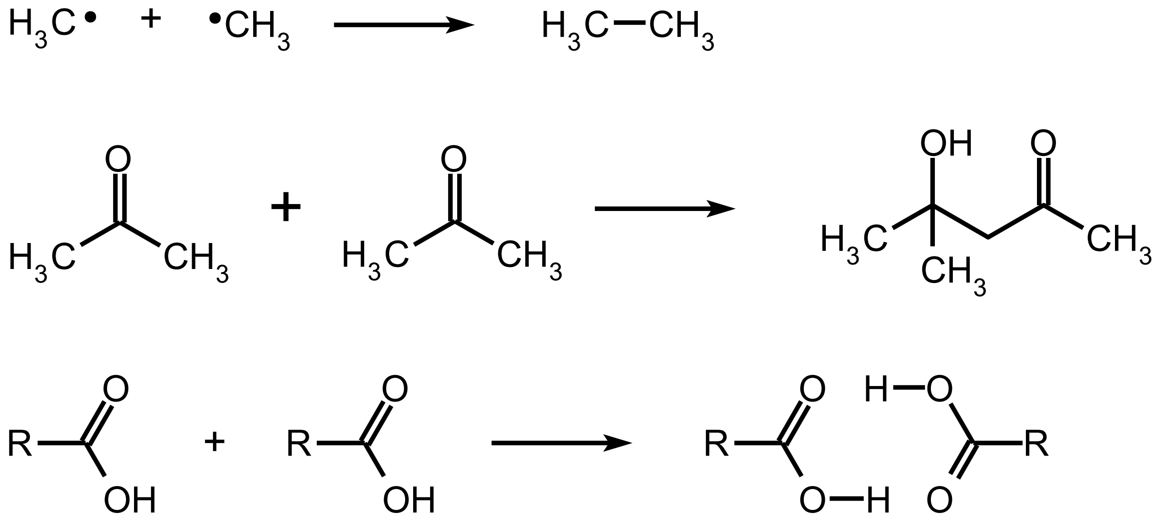
in mass spectrometry

An ion formed either when a chemical species exists in the vapour as a dimer and can be detected as such, or when a molecular ion can attach to a neutral molecule within the ion source to form an ion such as $[M_2]^{+\cdot}$ where M represents the molecule.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

dimerization

The transformation of a molecular entity A to give a molecular entity A_2. For example:

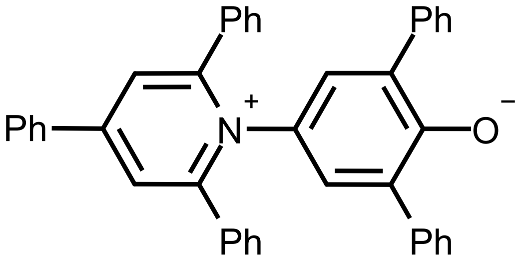


See also: association

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1106

Dimroth–Reichardt E_T parameter

A measure of the ionizing power (loosely polarity) of a solvent, based on the maximum wavenumber of the longest wavelength electronic absorption band of:



in a given solvent. E_T, called $E_T(30)$ by its originators, is given by:

$$E_T = 2.859 \times 10^{-3}\,\nu = 2.859 \times 10^{4}\,\lambda^{-1}$$

where E_T is in $\mathrm{kcal\ mol^{-1}}$, ν is in $\mathrm{cm^{-1}}$ and λ is in nm. The so-called normalized E_T^N scale is defined as:

$$E_T^N = \frac{E_T(\,\mathrm{solvent}\,) - E_T(\,\mathrm{Si\,Me_4})}{E_T(\,\mathrm{water}\,) - E_T(\,\mathrm{Si\,Me_4})} = \frac{E_T(\,\mathrm{solvent}\,) - 30.7}{32.4}$$

See also: Grunwald–Winstein equation, Z-value

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1106

diode laser

A solid state laser in which the active medium is the p-n junction between p-type and n-type semiconductor host materials. This term is preferred over the sometimes-used term semiconductor laser.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1920

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2236

diols

Compounds that contain two hydroxy groups, generally assumed to be, but not necessarily, alcoholic. Aliphatic diols are also called glycols.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

diosphenols

Cyclic α-diketones, which exist predominantly in an enolic form.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1332

dioxin

Colloquial (short) name of a toxic by-product (and sometimes contaminant) of herbicides; the full name of this species is: 2,3,7,8-tetrachlorodibenzo[*b,e*][1,4]-dioxin.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

dipolar aprotic solvent

A solvent with a comparatively high relative permittivity (or dielectric constant), greater than *ca*. 15, and a sizable permanent dipole moment, that cannot donate suitably labile hydrogen atoms to form strong hydrogen bonds, e.g. dimethyl sulfoxide. The term (and its alternative 'polar aprotic solvent') is a misnomer and is therefore discouraged. Such solvents are usually not aprotic but protophilic (and at most weakly protogenic). In describing a solvent it is better to be explicit about its essential properties, e.g. dipolar and non-protogenic.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1106

dipolar bond

A bond formed (actually or conceptually) by coordination of two neutral moieties, the combination of which results in charge-separated structures, e.g.

The term is preferred to the obsolescent synonyms 'coordinate link', 'coordinate covalence', 'dative bond', 'semipolar bond'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1106

dipolar compounds

Electrically neutral molecules carrying a positive and a negative charge in one of their major canonical descriptions. In most dipolar compounds the charges are delocalized; however the term is also applied to species where this is not the case. 1,2-Dipolar compounds have the opposite charges on adjacent atoms. The term 1,3-dipolar compounds is used for those in which a significant canonical resonance form can be represented by a separation of charge over three atoms (in connection with 1,3-dipolar cycloadditions). Subclasses of 1,3-dipolar compounds include:

1. Allyl type $X{=}Y^{+}{-}Z^{-} \longleftrightarrow X^{-}{-}Y^{+}{=}Z \longleftrightarrow X^{+}{-}Y{-}Z^{-} \longleftrightarrow X^{-}{=}Y{-}Z^{+}$ (X, Z = C, N, or O; Y = N or O)
   See: azo imides, azomethine imides, azomethine ylides, azoxy compounds, carbonyl imides, carbonyl oxides, carbonyl ylides, nitrones, nitro compounds
2. Propargyl type $X{\equiv}N^{+}{-}Z^{-} \longleftrightarrow X^{-}{=}N^{+}{=}Z \longleftrightarrow X^{-}{=}N{-}Z^{+} \longleftrightarrow X{-}N{=}Z$ (X = C or O, Z = C, N, or O)
   See: nitrile imides, nitrile oxides, nitrile ylides, nitrilium betaines, azides, diazo compounds
3. Carbene type $X{:}{-}C{=}Z \longleftrightarrow X^{+}{=}C{-}Z^{-}$ (X = C or N; Z = C, N, or O)
   See: acyl carbenes, imidoyl carbenes, vinyl carbenes
   See: betaines

   Source:
   PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1333

dipolar mechanism

of energy transfer

Synonymous with Förster excitation transfer
See also: energy transfer.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2236

dipole length

Electric dipole moment divided by the elementary charge.

Source:
Green Book, 2nd ed., p. 24

dipole moment

See: electric dipole moment

Source:
Green Book, 2nd ed., p. 24

dipole moment per volume

See: dielectric polarization

Source:
Green Book, 2nd ed., p. 14

dipole-induced dipole forces

See: van der Waals forces

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1107

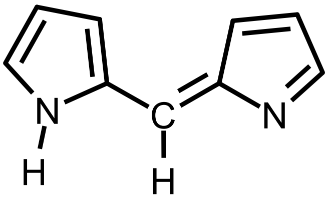
dipole–dipole interaction

Intermolecular or intramolecular interaction between molecules or groups having a permanent electric dipole moment. The strength of the interaction depends on the distance and relative orientation of the dipoles. The term applies also to intramolecular interactions between bonds having permanent dipole moments.
See also: van der Waals forces

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1106

dipyrrins

Compounds containing two pyrrole rings linked through a methine, –CH=, group.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1333

dipyrromethenes

See: pyrromethenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1333

diradicaloid

Synonym: biradicaloid

Diradical-like. Often used to refer to a species in which the two radical centres interact significantly.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 325

diradicals

Molecular species having two unpaired electrons, in which at least two different electronic states with different multiplicities [electron-paired (singlet state) or electron-unpaired (triplet state)] can be identified, e.g. $H_2C^{\cdot}–CH_2–C^{\cdot}H_2$ propane-1,3-diyl (trimethylene).
See also: biradical

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1333

direct amplification

A type of amplification reaction where the constituent to be determined is amplified directly and it is this constituent which is finally measured.

Source:
PAC, 1982, *54*, 2553 *(Recommendations on use of the term amplification reactions)* on page 2555

direct current

This term and its symbol, i_{dc} or I_{dc}, should be used (in preference to 'current' alone) only to denote the steady (time-dependent) component of a current that also has a periodic component.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1495

direct fission yield

The fraction of fissions giving rise to a particular nuclide before any nuclear decay has occurred.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

direct (radiochemical) isotope dilution analysis

Isotope dilution analysis used for the determination of a non-radioactive element with the aid of one of its radionuclides.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

direct reaction

Also contains definition of: impulsive reaction

A chemical process in which the reactive complex has a lifetime that is shorter than its period of rotation. In a molecular-beam experiment the reaction products of a direct reaction are scattered, with reference to the centre of mass of the system, in preferred directions rather than at random. Some direct reactions are impulsive which means that there is an energy exchange that is very fast compared to the vibrational time scale. A direct reaction is to be contrasted with an indirect reaction, also known as a complex-mode reaction.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 163

direct thermometric method [obsolete]

in enthalpimetric analysis

See: direct injection enthalpimetry

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2490

direct transfer gas flow system

in spectrochemical analysis

A system in which the purge gas transports the analyte directly to the sampling or excitation sources.

Source:
PAC, 1992, *64*, 261 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XIII. Terms related to chemical vapour generation (IUPAC Recommendations 1992))* on page 263

direct-injection burner (for analytical flame spectroscopy)

A burner in which oxidant and fuel emerge from separate ports and are mixed above the burner orifices through their turbulent motion.

Source:
Orange Book, p. 165

direct-injection enthalpimetry

Also contains definition of: batch injection calorimetry

An analytical method in which a reactant is injected into a calorimetric vessel containing another reagent. The enthalpy change of the ensuing reaction is measured and directly related to the amount of the limiting reagent (usually the analyte). If the experiment determines information other than amounts of analytes, an acceptable synonym is batch injection calorimetry. Other terms which have been used in the literature but are not recommended include the concentration thermometric technique and the direct thermometric method.

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2490

disaccharides

Compounds in which two monosaccharides are joined by a glycosidic bond.
See: saccharides, glycosides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1333

discomfort threshold

in atmospheric chemistry

The lowest value (e.g. concentration of an impurity, etc.) at which a sensation of discomfort is perceived; a measure which varies from person to person.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

discontinuous analyser

An analyser with at least one discontinuous subassembly.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

discontinuous indication

of an analyser

Indication related to the concentration during intervals of time which are not continuous.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

discontinuous measuring cell

A measuring cell which operates intermittently and not necessarily at fixed time intervals.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2178

discontinuous precipitation

A diffusional reaction in a multi-component system in which structural and compositional changes occur in regions immediately adjacent to the advancing interface. The parent phase remains unchanged until swept over by the interface; the transition is complete in regions over which the interface has passed. Synonymous with nucleation and growth.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 581

discontinuous simultaneous techniques

in analysis

The application of coupled techniques to the same sample when sampling for the second technique is discontinuous, e.g. discontinuous thermal analysis and gas chromatography, when discrete portions of evolved volatile(s) are collected from the sample situation in the instrument used for the first technique.

Source:
Orange Book, p. 39

discriminant analysis

Discriminant analysis is a statistical technique to find a set of descriptors which can be used to detect and rationalize separation between activity classes.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1142

discriminator

A basic function unit comprising an electronic circuit which gives an output pulse for each input pulse whose amplitude lies above a given threshold value.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1540

disintegration constant

See: decay constant

Source:
Green Book, 2nd ed., p. 22

See also:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 968

disintegration energy, Q

Energy liberated in a decay process and carried as kinetic energy of the emitted alpha or beta particle and the recoil energy of the product atom.

Source:
Green Book, 2nd ed., p. 22

disjoining pressure (for the attraction between two surfaces)

The force Π_d per unit area which can be obtained as the derivative of $-g_\mathrm{t}$ with respect to the distance, where g_t is the total Gibbs energy of interaction per unit area of each of the two flat and parallel plates.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 616

dispenser

A device used to deliver a measured amount of material.
See: sampler

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

dispersion (for spectroscopic instruments)

Dispersion of a material $= \frac{\mathrm{d}n}{\mathrm{d}\lambda}$ where n = refractive index and λ wavelength; angular dispersion $= \frac{\mathrm{d}\Phi}{\mathrm{d}\lambda}$ where Φ = angle; and linear dispersion $= \frac{\mathrm{d}x}{\mathrm{d}\lambda}$ where x = separation of spectral lines. The reciprocal of the last-named quantity is more frequently used ($\frac{\mathrm{d}\lambda}{\mathrm{d}x}$), and is commonly expressed in Å mm^{-1}.

Source:
Orange Book, p. 101

dispersion

in atmospheric chemistry

The dilution of a pollutant by spreading in the atmosphere due to diffusion or turbulent action (eddy diffusion).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

displacement chromatography

A procedure in which the mobile phase contains a compound (the displacer) more strongly retained than the components of the sample under examination. The sample is fed into the system as a finite slug.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 824
Orange Book, p. 74

displacive transition

A transition in which a displacement of one or more kinds of atoms or ions in a crystal structure changes the lengths and/or directions of bonds, without severing the primary bonds. Examples: The transitions of the low-temperature polymorphs of SiO_2 (quartz, tridymite and cristobalite) to their respective high-temperature polymorphs, which involve distortions or rotations of the SiO_4 tetrahedra. Also Jahn–Teller and ferroic transitions.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 581

disproportionation

Also contains definition of: radical disproportionation

Synonym: dismutation

1.

Any chemical reaction of the type

$$\mathrm{A} + \mathrm{A} \longrightarrow \mathrm{A'} + \mathrm{A''}$$

, where A, A' and A" are different chemical species. For example:

$$2\ \mathrm{ArH}^{+} \longrightarrow \mathrm{ArH} + \mathrm{ArH}_2^{+}$$

The reverse of disproportionation is called comproportionation. A special case of disproportionation (or 'dismutation') is 'radical disproportionation', exemplified by:

$$\mathrm{H_2\overset{\bullet}{C}{-}CH_3} + \mathrm{H_2\overset{\bullet}{C}{-}CH_3} \longrightarrow \mathrm{H_2C{=}CH_2} + \mathrm{H_3C{-}CH_3}$$

Reactions of the more general type:

$$\mathrm{R{-}\overset{\bullet}{C}H{-}CH_3} + \mathrm{R'{-}\overset{\bullet}{C}H{-}CH_3} \longrightarrow \mathrm{R{-}CH{=}CH_2} + \mathrm{R'{-}CH_2{-}CH_3}$$

are also loosely described as radical disproportionations.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1107
The following somewhat more restricted usage of the term prevails in inorganic chemistry.
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 581

2. A reversible or irreversible transition in which species with the same oxidation state combine to yield one of higher oxidation state and one of lower oxidation state.

Example:

$$3\ \mathrm{Au}^{+} \longrightarrow \mathrm{Au}^{3+} + 2\,\mathrm{Au}$$

The term also applies to an internal oxidation-reduction process as occurs, for example, among the iron atoms of $CaFeO_3$, where

$$2\,Fe^{4+} \longrightarrow Fe^{(4-\delta)+} + Fe^{(4+\delta)+}$$

, at Fe subarrays on lowering the temperature.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 581

disruptor

A chemical group used to disrupt the linearity of the backbone of molecules MCPLCs.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 504

dissociation

1. The separation of a molecular entity into two or more molecular entities (or any similar separation within a polyatomic molecular entity). Examples include unimolecular heterolysis and homolysis, and the separation of the constituents of an ion pair into free ions.
2. The separation of the constituents of any aggregate of molecular entities.

In both senses dissociation is the reverse of association.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1107

dissociation energy, E_d, D

Energy required to dissociate a molecule into two parts. Subscripts 0 and e, i.e. D_0 and D_e, are used to denote the dissociation from the ground state and potential energy minimum, respectively.
See also: bond-dissociation energy

Source:
Green Book, 2nd ed., p. 20

dissociative adsorption (dissociative chemisorption)

Also contains definition of: associative desorption

Adsorption with dissociation into two or more fragments, both or all of which are bound to the surface of the adsorbent The process may be homolytic, as in the chemisorption of hydrogen:

$$H_2 + 2\,* \rightarrow 2H^*$$

where * represents a surface site, or heterolytic, as in:

$$H_2 + M^{n+} + O^{2-} \rightarrow H^{-}M^{n+} + HO^{-}$$

where M^{n+} and O^{2-} are surface sites in which the ions are of lower coordination than the ions in the bulk phase. Associative desorption is the reverse of dissociative adsorption.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 84

dissociative ionization

in mass spectrometry

An ionization process in which a gaseous molecule decomposes to form products, one of which is an ion.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

dissociative surface reaction

Also contains definition of: associative surface reaction

Dissociative surface reaction and its reverse, associative surface reaction, are defined by:

$$2\,* + C_2H_5^* \rightleftharpoons H^* + {}^*CH_2CH_2^*$$

where * represents a surface site.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 84

dissolution

The mixing of two phases with the formation of one new homogeneous phase (i.e. the solution).

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 581
Orange Book, p. 83

dissymmetry [obsolete]

in stereochemistry

Obsolescent synonym for chirality.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2206

dissymmetry of scattering

The ratio of two Rayleigh ratios for different angles of observation, i.e.

$$z(\theta_1, \theta_2) = \frac{R(\theta_1)}{R(\theta_2)}$$

$$\theta_1 < \theta_2$$

The angles must be specified; in light scattering it is customary to let $\theta = 180\,° - \theta_1$ and, most frequently, $\theta_1 = 45\,°$ and $\theta_2 = 135\,°$.

Source:
Purple Book, p. 67

See also:
PAC, 1983, *55*, 931 *(Definitions, terminology and symbols in colloid and surface chemistry. Part 1.14: Light scattering (Provisional))* on page 932

distonic radical cation

A radical cation in which charge and radical sites are separated.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1107

distribuend

The substance that is distributed between two immiscible liquids or liquid phases.

Source:
Orange Book, p. 91

distribution

The apportionment of a solute between two phases. The term partition or extraction may also be used in this sense where appropriate.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2377

distribution coefficient

See: distribution constant, distribution ratio
The term is not recommended as a synonym for the latter.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2381

distribution constant

Synonymous with partition ratio.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2381

distribution constant

in chromatography

The concentration of a component in or on the stationary phase divided by the concentration of the component in the mobile phase. Since in chromatography a component may be present in more than one form (e.g. associated and dissociated forms), the analytical condition used here refers to the total amount present without regard to the existence of various forms. These terms are also called the distribution coefficients. However, the present term conforms more closely to the general usage in science.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 847

See also:
Orange Book, p. 88
Orange Book, p. 106
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 969

distribution function

in polymers

A normalized function giving the relative amount of a portion of a polymeric substance with a specific value, or a range of values, of a random variable or variables.
Notes:

1. Distribution functions may be discrete, i.e. take on only certain specified values of the random variable(s), or continuous, i.e. take on any intermediate value of the random variable(s), in a given range. Most distributions in polymer science are intrinsically discrete, but it is often convenient to regard them as continuous or to use distribution functions that are inherently continuous.
2. Distribution functions may be integral (or cumulative), i.e. give the proportion of the population for which a random variable is less than or equal to a given value. Alternatively they may be differential distribution functions (or probability density functions), i.e. give the (maybe infinitesimal) proportion of the population for which the random variable(s) is (are) within a (maybe infinitesimal) interval of its (their) range(s).
3. Normalization requires that: (i) for a discrete differential distribution function, the sum of the function values over all possible values of the random variable(s) be unity; (ii) for a continuous differential distribution function, the integral over the entire range of the random variable(s) be unity; (iii) for an integral (cumulative) distribution function, the function value at the upper limit of the random variable(s) be unity.

Source:
Purple Book, p. 55

distribution isotherm

in chromatography

The equilibrium relation between the concentration of a sample component in the stationary phase c_{S}, and in the mobile phase c_{M}, expressed as a function $c_{\mathrm{S}} = f(c_{\mathrm{M}})$.
Note:
The relation can be influenced also by concentrations of other sample components. c_{S} and c_{M} are usually expressed per unit volume of the phase; c_{S} may also be expressed per mass of the dry solid phase or per unit surface area.
In some versions of chromatography, a distribution isotherm can be seen as a partition isotherm, an adsorption isotherm, or a combination of these, depending on the mechanism of separation.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1592
This definition supersedes an earlier definition of distribution isotherm *in chromatography*.

distribution ratio, *D*

in liquid-liquid distribution

The ratio of the total analytical concentration of a solute in the extract (regardless of its chemical form) to its total analytical concentration in the other phase.
Notes:
1. If there is possible confusion with the extraction factor or (mass) distribution ratio the term concentration distribution ratio (symbol D_{c}) should be used, but this is not common usage. This is reasonably compatible with chromatographic nomenclature.
2. The terms distribution coefficient, extraction coefficient and, where appropriate, scrubbing coefficient, stripping coefficient are widely used alternatives but are not recommended. If they must be used in a given situation the term ratio is preferable to coefficient.

3. In equations relating to aqueous/organic systems the organic phase concentration is, by convention, the numerator and the aqueous phase concentration the denominator. In the case of stripping ratio the opposite convention is sometimes used but should then be clearly specified.
4. In the past there has been much confusion between the distribution ratio as defined above, the value of which varies with experimental conditions, e.g. pH, presence of complexing agents, extent of achievement of equilibrium etc. and the true partition coefficient which is by definition invariable or the partition coefficient or distribution constant which apply to a particular chemical species under specified conditions. For this reason the terms distribution constant, partition constant, partition coefficient, partition ratio and extraction constant should not be used in this context.
5. The use of the ratio: light phase concentration to heavy phase concentration is ambiguous and is not recommended.
6. The distribution ratio is an experimental parameter and its value does not necessarily imply that distribution equilibrium between the phases has been achieved.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2382
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 970
Orange Book, p. 89

disyndiotactic polymer

A syndiotactic polymer that contains two chiral or prochiral atoms with defined stereochemistry in the main chain of the configurational base unit.

Source:
Purple Book, p. 32

ditactic polymer

A tactic polymer that contains two sites of defined stereoisomerism in the main chain of the configurational base unit.

Source:
Purple Book, p. 32

diterpenoids

Terpenoids having a C_{20} skeleton.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1333

diurnal variation

in atmospheric chemistry

Indicates variations which follow a distinctive pattern which recurs with a daily cycle.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

dividing surface

A surface, usually taken to be a hyperplane, constructed at right angles to the minimum-energy path on a potential-energy surface. In conventional transition-state theory it passes through the highest point on the minimum-energy path. In generalized versions of transition-state theory the dividing surface can be at other positions; in variational transition-state theory the position of the dividing surface is varied so as to get a better estimate of the rate constant.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 163

DM-interference

Interference in which the analytical signal is influenced by a different mechanism than the analyte e.g. the formation of non-dissociating species in emission spectroscopy.

Source:
PAC, 1983, *55*, 553 *(Recommendations for the usage of selective, selectivity and related terms in analytical chemistry)* on page 554

DNA probe

A short sequence of DNA labelled isotopically or chemically that is used for the detection of a complementary nucleotide sequence.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 152

Dobson unit

in atmospheric chemistry

Unit sometimes used in the description of the total ozone in a column of air overhead. It is given as the thickness (in units of 10^{-3} cm or 10^{-5} m) of that layer which would be formed by the total ozone in a column reduced to the pressure of 760 Torr and temperature of 0 °C.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

docking studies

Docking studies are computational techniques for the exploration of the possible binding modes of a substrate to a given receptor, enzyme or other binding site.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1142

dodecahedro-

An affix used in names to denote eight atoms bound into a dodecahedron with triangular faces.

Source:
Red Book, p. 245
Blue Book, p. 464

dolichols

A group of prenol derivatives in which n in the general formula H–[CH_2–C(CH_3)=CH–CH_2]$_n$–OH is greater than 4 and in which the residue that carries the hydroxy group is saturated, i.e. 2,3-dihydropolyprenols.
Note:
The collective term prenol should not be used without qualification to include dolichols since these are derivatives of prenols.

Source:
White Book, p. 255

Donnan emf (Donnan potential)

The potential difference E_{D} at zero electric current between two identical salt bridges, usually saturated KCl bridges (conveniently measured by linking them to two identical electrodes) inserted into two solutions in Donnan equilibrium.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 619

Donnan equilibrium

The equilibrium characterized by an unequal distribution of diffusible ions between two ionic solutions (one or both of the solutions may be gelled) separated by a membrane which is impermeable to at least one of the ionic species present, e.g. because they are too large to pass through the pores of the membrane. The membrane may be replaced by other kinds of restraint, such as gelation, the field of gravity, etc., which prevent some ionic components from moving from one phase to the other, but allow other components to do so.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 619

Donnan exclusion

Reduction in concentration of *mobile* ions within an ion exchange membrane due to the presence of *fixed* ions of the same sign as the mobile ions.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1488

donor number (DN)

A quantitative measure of Lewis basicity.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1107

dopant

Charge-transfer agent used to generate, by oxidation or reduction, positive or negative charges in an intrinsically conducting polymer.
Note:
Examples of dopants include AsF_5 or I_2 as oxidizing agents, generating cation radicals on the chains of an intrinsically conducting polymer (so-called holes), or a solution of sodium naphthalenuidyl in tetrahydrofuran as a reducing agent, generating anion radicals on the chains of an intrinsically conducting polymer.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2069

doping

in catalysis

The action of adding a small amount of foreign atoms to form a solid solution in the lattice of a non-metallic catalyst.

Source:
PAC, 1991, *63*, 1227 *(Manual on catalyst characterization (Recommendations 1991))* on page 1231

doping

in polymer chemistry

Oxidation or reduction process brought about by a dopant.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2070

Doppler broadening

of a spectral line

Broadening due to the random motion of the emitting or absorbing atoms. A Doppler broadened line has a Gaussian shape.

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1463

dosage

in atmospheric chemistry

As applied to an air pollutant in an exposure chamber, dosage is commonly defined as the concentration of the pollutant times the duration of exposure.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

dose

Energy or amount of photons absorbed per volume (or per mass) by an irradiated object during a particular exposure time. SI units are $\mathrm{J\ m^{-3}}$ or $\mathrm{J\ g^{-1}}$ and $\mathrm{mol\ m^{-3}}$ or $\mathrm{mol\ g^{-1}}$, respectively. Common units are $\mathrm{einstein\ m^{-3}}$ or $\mathrm{einstein\ g^{-1}}$, respectively.
Note:
In medicine and in some other research areas (e.g., photopolymerization and water purification through irradiation) dose is used in the sense of exposure, i.e., the energy or amount of photons per surface area (or per volume) impinging upon an irradiated object during a particular exposure time. This use is not recommended. The terms photon exposure and radiant exposure are preferred.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 326
See also: UV dose, einstein
This definition supersedes an earlier definition of dose.

dose equivalent, *H*

Product of the absorbed dose of ionizing radiation, a quality factor and a modifying factor to take into account the effect of radiation on different biological tissues.

Source:
Green Book, 2nd ed., p. 72
ISO 31-10: 1992 *(Quantities and Units - Part 10: Nuclear Reactions and Ionizing Radiations.)*
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 970

dose

in radioanalytical chemistry

A general term denoting the quantity of radiation or energy absorbed. For special purposes, it must be appropriately qualified e.g. absorbed, maximum permissible, mean lethal.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1540

dose

of a substance

Total quantity of a substance administered to, taken up, or absorbed by an organism, organ, or tissue.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1049

dose-response and dose-effect relationships

The graph of the relation between dose and the proportion of individuals responding with an all-or-none effect; it is essentially the graph of the probability of an occurrence (or the proportion of a population exhibiting an effect) against dose. Typical examples of such all-or-none effects are mortality or the incidence of cancer.

The dose-effect curve is the graph of the relation between dose and the magnitude of the biological change produced measured in appropriate units. It applies to measurable changes giving a graded response to increasing doses of a drug or xenobiotic. It represents the effect on an individual animal or person, when biological variation is taken into account. An example is the increased effect of lead on the haem synthesis, *e.g.*, on activity of the enzyme 6-amino laevulinic acid dehydratase in blood serum or coproporphyrin levels in urine.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1022

double escape peak

In a gamma-ray spectrum, the peak due to pair production in the detector and escape, from the sensitive part of the detector, of two photons of $511\ \mathrm{keV}$ resulting from annihilation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

double-beam spectrometer (for luminescence spectroscopy)

Double (spectral) beam spectrometers are used where two samples are to be excited by two different wavelengths. A double- (synchronous) beam spectrometer is a luminescence spectrometer in which both the excitation and emission monochromators scan the excitation and emission spectra simultaneously, usually with a fixed wavelength difference between excitation and emission.

Source:
Orange Book, p. 191

double-focusing mass spectrograph

An instrument which uses both direction and velocity focusing, and therefore an ion beam initially diverging in direction and containing ions of different kinetic energies is separated into beams according to the quotient mass/charge, these beams being focused on to a photographic plate or film.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545

double-focusing mass spectrometer

An instrument which uses both direction and velocity focusing, and therefore an ion beam of a given mass/charge is brought to a focus when the ion beam is initially diverging and contains ions of the same mass and charge with different translational energies. The ion beam is measured electrically.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545
Orange Book, p. 201

double-layer current

The non-faradaic current associated with the charging of the electrical double layer at an electrode-solution interface, given by:

$$i_{\mathrm{DL}} = \frac{\mathrm{d}(\sigma\, A)}{\mathrm{d}t}$$

where σ = surface charge density of the double layer, A = area of the electrode-solution interface and t = time. Capital letters should be used as subscripts to avoid the possibility of confusing this symbol with that for the limiting diffusion current.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1496

double-strand chain

in polymers

A chain that comprises constitutional units connected in such a way that adjacent constitutional units are joined to each other through three or four atoms, two on one side and either one or two on the other side of each constitutional unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2294

double-strand copolymer

A copolymer the macromolecules of which are double-strand macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2304

double-strand macromolecule

A macromolecule that comprises constitutional units connected in such a way that adjacent constitutional units are joined to each other through three or four atoms, two on one side and either one or two on the other side of each constitutional unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2295

double-strand polymer

Also contains definitions of: ladder polymer, spiro polymer

A polymer the macromolecules of which are double-strand macromolecules.
Notes:

1. A polymer, the macromolecules of which are spiro macromolecules is termed a spiro polymer.
2. A polymer, the macromolecules of which are ladder macromolecules is termed a ladder polymer.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2304

double-wavelength spectroscopy

The effect of spectral background due to impurities, solvent or radiation scattering may be reduced if the difference in the absorbances of a sample measured at two selected wavelengths is obtained. This is often achieved by repetitively switching from one wavelength to the other. Double-wavelength spectroscopy does this automatically by allowing two beams of radiation of different wavelengths to pass through the cell. One beam is fixed at a longer wavelength and the other measures absorbance while being scanned over a limited wavelength range at shorter wavelengths.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1455

doublet state

A state having a total electron spin quantum number equal to $\frac{1}{2}$.
See: multiplicity

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2237

doubling time t_D

in biotechnology

The time (min, h) required for a cell population to double either the number of cells or the active cell mass.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 152

down-time

in analysis

The loss of time that should be available for analysis. This might be due to breakdown, maintenance or other factors.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663

downconversion

Process by which a photon with frequency ν_1 interacts with a non-linear medium and splits into two simultaneously emitted photons with frequencies ν_2 and ν_3 so that the energy is conserved:

$$\nu_1 = \nu_2 + \nu_3$$

Notes:

1. Also known as a parametric downconversion.
2. The efficiency of the conversion process depends on the parametric gain in the non-linear material. This in turn depends on the power of the incident radiation, the photon frequencies, their indices of refraction in the material, and the non-linear 'hyper-susceptibility' of the material.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 326

downfield

See: chemical shift

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1107

downstream

in membrane processes

Side of a membrane from which permeate emerges.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1482

downwash

in atmospheric chemistry

As applied to the action of chimney gases, it is the downward motion of the chimney gases brought on by eddies which form in the lee of a chimney when the wind is blowing. It may result in bringing the flue gases to the ground prematurely.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

drift

A slow non-random change in signal with time.
See also: noise

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663

driving force (affinity) of a reaction, A

The decrease in Gibbs energy on going from the reactants to the products of a chemical reaction ($-\Delta G$).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1107

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2237

driving force (for electron transfer)

Term widely used to indicate the negative of the standard Gibbs energy change for outer-sphere electron transfer ($\Delta_{\mathrm{ET}}G^{\mathrm{o}}$).

Note:
For photo-induced processes, this quantity can often be estimated from independently determined properties of the donor and acceptor species involved using the equation for the calculation of the Gibbs energy of photo-induced electron transfer.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 327

drop time

in polarography

The time that elapses between the instants at which two successive drops of liquid metal are detached from the tip of the capillary.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1500

droplet

in atmospheric chemistry

A small liquid particle. The size of droplets encountered in the atmosphere extends over a wide range; e.g. liquid aerosol solutions which make up the fine particle fraction of continental tropospheric aerosol are usually $2\ \mu\mathrm{m}$ in diameter. Cloud water droplets usually have diameters in the range of $5 - 70\ \mu\mathrm{m}$, while rain droplets commonly have diameters ranging from $0.1 - 3\ \mathrm{mm}$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

Drude–Nernst equation (for electrostriction)

Equation describing the contraction (ΔV_{el}) taking place in a dielectric medium of relative static permittivity ε_{r} (formerly called dielectric constant) upon introduction of an ion of charge number z and radius r:

$$\Delta V_{\mathrm{el}} = -\frac{(z\,e)^2}{2\,r\,\varepsilon_{\mathrm{r}}}\frac{\partial(\ln\varepsilon_{\mathrm{r}})}{\partial p}$$

with e the elementary charge.
Note:
Inasmuch as the derivative of $\ln\varepsilon_{\mathrm{r}}$ with respect to pressure, $\frac{\partial(\ln\varepsilon_{\mathrm{r}})}{\partial p}$, is not known for all media, there are approximations to evaluate this term as a function of ε_{r} and of the isothermal compressibility of the medium, κ_T.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 327

drug

Any substance which when absorbed into a living organism may modify one or more of its functions. The term is generally accepted for a substance taken for a therapeutic purpose, but is also commonly used for abused substances. Synonymous with medicine, pharmaceutical.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2040

drug design

Drug design includes not only ligand design, but also pharmacokinetics and toxicity, which are mostly beyond the possibilities of structure- and/or computer-aided design. Nevertheless, appropriate chemometric tools, including experimental design and multivariate statistics, can be of value in the planning and evaluation of pharmacokinetic and toxicological experiments and results. Drug design is most often used instead of the correct term 'Ligand Design'.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1142

dry bulb temperature

in atmospheric chemistry

In psychrometry, the temperature of the gas measured by a dry bulb thermometer.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

drying agent

A substance which removes water (liquid or gaseous).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

drying control chemical additive

Acronym: DCCA

Co-solvent included to facilitate the rapid drying of gels without cracking.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1809

dual fluorescence

of systems or molecular species

Systems or molecular species showing two fluorescence bands. Several non-trivial molecular properties may be at the basis of a dual fluorescence, such as conformational equilibrium in the ground state and a mixture of excited states.
Note:
Trivial reason for dual fluorescence is the coexistence of two independent fluorophores.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 327

dual substituent-parameter equation

In a general sense, any equation which expresses substituent effects in terms of two parameters. However, in practice the term is used more specifically for an equation for summarizing the effects of *meta*- or *para*- substituents (i = m or p) **X** on chemical reactivity, spectroscopic properties, etc. of a probe site **Y** in benzene or other aromatic system.

$$P^i = \rho_I^i \sigma_I + \rho_R^i \sigma_R$$

P is the magnitude of the property **Y** for substituent **X**, expressed relative to the property for X = H; σ_I and σ_R are inductive or polar and resonance substituent constants, respectively, there being various scales for σ_R; ρ_I and ρ_R are the corresponding regression coefficients.

See also: extended Hammett equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1107

dual-mode photochromism

Photochromism occurring in complex systems and triggered alternatively by two different external stimuli, such as light and an electric current. In such a case photochromism and 'electrochromism' are mutually regulated.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 327

dust collector

in atmospheric chemistry

A device for monitoring dust emissions. Also the equipment used to remove and collect dust from process exhaust gases; this may employ simply sedimentation (dustfall jars, coated slides, papers, etc.), inertial separation (cyclones, impactors, impingers, etc.), precipitation (thermal and electrostatic) or filtration.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

dust fall

in atmospheric chemistry

Solid particles in the air which fall to the ground under the influence of gravity.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

dust

in atmospheric chemistry

Small, dry, solid particles projected into the air by natural forces, such as wind, volcanic eruption and by mechanical or manmade processes such as crushing, grinding, milling, drilling, demolition, shoveling, conveying, screening, bagging and sweeping. Dust particles are usually in the size range from about $1 - 100\ \mu\mathrm{m}$ in diameter and they settle slowly under the influence of gravity.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

dye laser

A CW or pulsed source of coherent radiation in which the active medium is usually a solution of a fluorescent organic molecule (the dye) pumped with a suitable pump laser or with a flash lamp. These lasers can be tuned over a large part of the fluorescence band of the dye.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2237

dynamic field(s) mass spectrometer

A mass spectrometer in which the separation of a selected ion beam depends essentially on the use of fields, or a field, varying with time. These fields are generally electric.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545
Orange Book, p. 202

dynamic membrane formation

Process in which an active layer is formed on the membrane surface by the deposition of substances contained in the fluid being treated.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1482

dynamic range

of an analyser

The ratio between the maximum usable indication and the minimum usable indication (detection limit). A distinction may be made between the linear dynamic range, where the response is directly proportional to concentration, and the dynamic range where the response may be non-linear, especially at higher concentrations.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2185

dynamic reaction path (DRP)

A classical trajectory method based on molecular orbital calculations which determines atomic accelerations, velocities and positions using the energy gradient, and does not require prior knowledge of the potential energy surface.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1935

dynamic surface tension

Synonym: dynamic interfacial tension

In certain circumstances, one may measure surface tensions that are different from the equilibrium value. Such a surface tension is called the dynamic surface (or interfacial) tension (γ^{dyn} or σ^{dyn}). The equilibrium value is then called the static surface (or interfacial) tension (γ^{st} or σ^{st}). The modifying signs may be omitted if there is no danger of ambiguity.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 597

dynamic thermomechanometry

A technique in which the dynamic modulus and/or damping of a substance under oscillatory load is measured as a function of temperature while the substance is subjected to a controlled temperature program.

Source:
Orange Book, p. 45

dynamic viscosity, η

For a laminar flow of a fluid the ratio of the shear stress to the velocity gradient perpendicular to the plane of shear.
See also: viscosity

Source:
Green Book, 2nd ed., p. 13

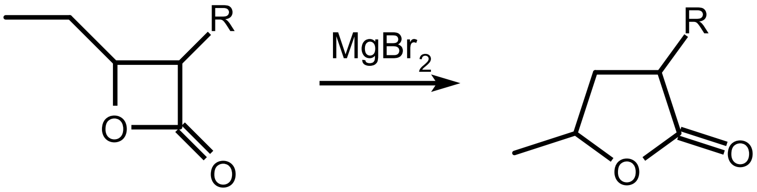
dyne

cgs unit of force, $\mathrm{dyn} = 10^{-5}\,\mathrm{N}$.

Source:
Green Book, 2nd ed., p. 112

dyotropic rearrangement

An uncatalysed process in which two σ-bonds simultaneously migrate intramolecularly, e.g.



Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1108

dypnones

1,3-Diphenylbut-2-en-1-one, $PhC(=O)CH=C(CH_3)Ph$, and its ring-substituted derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1333

η (eta or hapto)

in inorganic nomenclature

An affix giving a topological indication of the bonding between a π-electron ligand and the central atom in a coordination entity. A right superscript numerical index indicates the number of ligating atoms in the π-electron system of the ligand which bind to the central atom. Examples:

1. $[Fe(CO)_3(C_4H_6SO)]$, tricarbonyl(η^2-dihydrothiophene 1-oxide-κ*O*)iron.
2. $[Cr(CO)_4(C_4H_6)]$, tetracarbonyl(η^4-2-methylene-1,3-propanediyl)chromium.

Source:
Red Book, p. 202

See also:
Blue Book, p. 465
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120

E, *Z*

The approved stereodescriptors of stereoisomeric alkenes $R^1R^2C=CR^3R^4$ ($R^1 \neq R^2$, $R^3 \neq R^4$); neither R^1 nor R^2 need be different from R^3 or R^4), cumulenes $R^1R^2C(=C=C)_n=CR^3R^4$ and related systems e.g. $R^1R^2C=NOH$, $HON=C\{[CH_2]_n\}_2C=NOH$. The group of highest CIP priority attached to one of the terminal doubly bonded atoms of the alkene, oxime, etc. or cumulene (i.e. R^1 or R^2) is compared with the group of highest precedence attached to the other (i.e. R^3 or R^4). The stereoisomer is designated as *Z* (zusammen = together) if the groups lie on the same side of a reference plane passing through the double bond and perpendicular to the plane containing the bonds linking the groups to the double-bonded atoms; the other stereoisomer is designated as *E* (entgegen = opposite). The descriptors may be applied to structures with a fractional bond order between one and two; and to double bonds involving elements other than carbon. They are not used to describe ring substitution relationships.
See also: *cis-trans* isomers

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2206

E/*Z* photoisomerization

General designation of a photoinduced geometrical isomerization of a C–C double bond.
Note:
Geometrical isomerization of a C–C double bond is called a *cis/trans isomerization* in 1,2-disubstituted alkenes.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 338

$\frac{E}{2}$mass spectrum

Processes of the charge-stripping type:

$$\mathrm{M}^{+} + \mathrm{X} \rightarrow \mathrm{M}^{2+} + \mathrm{X} + \mathrm{e}$$

occuring in a collision cell (containing a gas, X) located in a field-free region preceding a magnetic and electric sector combination placed in either order, may be detected as follows. If the instrument slits are wide and if the electric sector field E is set to half the value required to transmit the main ion-beam, the only ions to be transmitted will be those with a kinetic energy/charge ratio half, or almost exactly half, that of the main ion beam. The product ions of the charge-stripping process fulfil this condition. If the magnetic field B is scanned, a mass spectrum of such doubly-charged product ions, and thus of their singly-charged precursors, is obtained. Such a spectrum is called an $\frac{E}{2}$ mass spectrum. Interference from product ions from processes of the type:

$$\mathrm{M}_1^{+} + \mathrm{X} \rightarrow \mathrm{M}_2^{+} + \mathrm{X} + \mathrm{M}_3$$

where m_1, m_2, and $(m_1 - m_2)$ are the masses of M_1^{+}, M_2^{+} and M_3, respectively, and where $m_2 = 0.5\ m_1$, can arise in $\frac{E}{2}$ mass spectra.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1552

eclipsed (eclipsing)

Two atoms or groups attached to adjacent atoms are said to be eclipsed if the torsion angle between the three bonds is zero (or approximately so).
See: bisecting conformation, eclipsing strain

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2206

eclipsing strain

Synonyms: bond opposition strain, Pitzer strain, torsional strain

Intramolecular strain present due to nonbonded interactions between two eclipsed atoms or groups. It is, for example, one of the interactions responsible for the existence of a rotational barrier and hence restricted rotation about the C–C bond in ethane. It has also been called Pitzer strain, torsional strain and bond opposition strain.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2206

eddy

In turbulent fluid motion, a blob of the fluid that has some definitive character and moves in some way differently from the main flow.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

eddy dispersion (diffusion)

The process by which substances are mixed in the atmosphere or in any fluid system due to eddy motion.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

educt [obsolete]

Term used mainly in the German literature for starting material (reactant). It should be avoided in English, because there it means 'something that comes out' and not 'something that goes in'. The German use of the term is in fact also incorrect.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1108

effective cadmium cut-off energy

in nuclear analytical chemistry

In a given experimental configuration, the energy value determined by the condition that the detector response would be unchanged if the cadmium cover surrounding the detector was replaced by a fictitious cover opaque to neutrons with energy below this value and transparent to neutrons with energy above this value.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1540
Orange Book, p. 221

effective charge

Change in effective charge is a quantity obtained by comparison of the polar effect of substituents on the free energies of rate or equilibrium processes with that on a standard ionization equilibrium. Provided the effective charges on the states in the standard equilibrium are defined, then it is possible to measure effective charges for states in the reaction or equilibrium under consideration.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1108

effective chimney height (stack height)

A height used for the purposes of calculating the dispersion of emitted gases from a chimney, and which differs from the real chimney height by an amount which depends on such factors as the exit velocity, buoyancy effects and wind speed; it may also be affected by the local topography. It denotes the maximum height of the centre of a plume path above the level of the ground. The effective height may be above or below the actual chimney height, although the former case is most common.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2179

effective half life

For a radioactive substance, the time required for the amount of that substance in a biological system to be reduced to one half of its value by both radioactive decay and biological processes, when the rate of removal is approximately exponential.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

effective molarity (effective concentration)

The ratio of the first-order rate constant of an intramolecular reaction involving two functional groups within the same molecular entity to the second-order rate constant of an analogous intermolecular elementary reaction. This ratio has the dimension of concentration. The term can also apply to an equilibrium constant.
See also: intramolecular catalysis

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1108

effective theoretical plate number

of a chromatographic column

A number indicative of column performance when resolution is taken into account:

$$N = \frac{16\, R_\mathrm{s}^{\,2}}{(1-\alpha)^2}$$

where R_s is the peak resolution and α is the separation factor.
See also: plate number *in chromatography*

Source:
Orange Book, p. 108

effective thermal cross-section

A fictitious cross-section for a specified reaction, which, when multiplied by the 2200 metre-per-second flux density, gives the correct reaction rate for thermal neutrons.
See also: microscopic cross-section

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517
Orange Book, p. 218

effectively infinite thickness

in flame spectroscopy

Solid or liquid samples of one gram or more are generally used in X-ray spectroscopy. If the sample is thick enough so that the intensity of characteristic fluorescent radiation is not significantly modified by an increase in thickness, the sample is described as a bulk sample of effectively infinite thickness.

Source:
Orange Book, p. 182

effectiveness

See: spectral (photon) effectiveness

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2237

effector

A small molecule which increases (activator) or decreases (inhibitor) the activity of an (allosteric) protein by binding to the protein at the regulatory site (which is different from the substrate-binding catalytic site).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 152

efficiency, η

of a step

The ratio between the useful energy delivered or bound and the energy supplied, i.e. energy output/ energy input. It is also used in the sense of a quantitative measure of the relative rate of a given step involving a species with respect to the sum of the rates of all of the parallel steps which depopulate that species.
See also: quantum yield

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2238

efficiency of atomization

in analytical flame spectroscopy

The ratio of the amount of analyte that passes through the flame cross-section at the observation height, as free neutral (or ionized) atoms, to the amount of analyte aspirated.

Source:
Orange Book, p. 124

efficiency of nebulization, ε_{n}

in flame spectrometry

The substance fraction of component entering the flame in the amount of component consumed. The efficiency of nebulization is related to the amount of component and not to the amount of solvent. It cannot be calculated directly from the ratio: volume rate of sample drained from the spray chamber divided by volume rate of fluid consumed. Corrections usually have to be made to take account of differences in component concentrations in the drained and consumed solutions, respectively, because of evaporation of some solvent from mist droplets deposited on the walls.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1740
Orange Book, p. 168

efficiency spectrum

A plot of the efficiency of a step (η) against wavelength or photon energy.
See: action spectrum, conversion spectrum
See also: spectral effectiveness

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2238

efflorescence

The reverse of deliquescence: the drying of a salt solution when the vapour pressure of water in the saturated solution of a substance is greater than the partial pressure of water in the ambient air. Also refers to the loss of water of crystallization from a solid salt such as $Na_2CO_3{\cdot}10H_2O$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

effluent

Any spent liquors or other waste materials which are emitted by a source (waste from plating shops, pickling tanks, sewage treatment plants, chemical manufacturing plants, etc.).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

effluent

in chromatography

The mobile phase leaving the column.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 824

eighteen-electron rule

An electron-counting rule to which an overwhelming majority of stable diamagnetic transition metal complexes adhere. The number of nonbonded electrons at the metal plus the number of electrons in the metal-ligand bonds should be 18. The 18 electron rule in transition metal chemistry is a full analogue of the 'Lewis octet rule'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1108

einstein [obsolete]

One mole of photons. Although widely used, it is not an IUPAC sanctioned unit. It is sometimes defined as the energy of one mole of photons. This use is discouraged.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2238

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

Einstein equation

In its most general form, the Einstein equation relates the atomic mobility b_i of a species i to the diffusion coefficient D_i: i.e., $D_i = k\,T\,b_i$.

Source:
PAC, 1999, *71*, 1307 *(Definitions of Terms for Diffusion in the Solid State)* on page 1314

El-Sayed rules

The rate of intersystem crossing is relatively large if the radiationless transition involves a change of orbital type.
Note:
A typical case is the transition from the lowest *singlet state* to the *triplet manifold*, *e.g.*, $^1\pi,\pi^* \rightarrow {}^3n,\pi^*$ is faster than $^1\pi,\pi^* \rightarrow {}^3\pi,\pi^*$ and $^1n,\pi^* \rightarrow {}^3\pi,\pi^*$ is faster than $^1n,\pi^* \rightarrow {}^3n,\pi^*$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 331

elastic collision

Also contains definition of: inelastic collision

A particle (atom or molecule) can undergo a change in its state of excitation as a result of collisions with other particles. In an elastic collision an exchange only of kinetic energy takes place between the colliding species; in an inelastic collision there is an interchange between the kinetic energy and the internal energy of the particle.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 159

elastic scattering

in reaction dynamics

When in a molecular collision there is no transfer of energy among different degrees of freedom, there is said to be elastic scattering.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 163
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1540

elastic scattering

in spectrochemistry

Radiation may be scattered by its transmission through a medium containing particles. If the scatter results in no significant change in the wavelength relative to the primary radiation it is called elastic scattering. In cases where the scattering centres are small compared to the wavelength of the radiation the elastic scattering is called Rayleigh scattering and Mie scattering if this condition is not fulfilled.

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1464

elastically active network chain

Segment of a chain between two successive crosslinks in a polymer network that is long enough to show entropic elasticity.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1819

elastomer

Polymer that displays rubber-like elasticity.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1810

electric capacitance

See: capacitance

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 970

electric charge, Q

Integral of the electric current over time. The smallest electric charge found on its own is the elementary charge, e, the charge of a proton.

Source:
Green Book, 2nd ed., p. 14
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 970

electric conductance, G

Reciprocal of the electric resistance.

Source:
Green Book, 2nd ed., p. 15
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 970

electric conductivity

See: conductivity

Source:
Green Book, 2nd ed., p. 15
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 970

electric current, I

Base quantity in the system of quantities upon which SI is based.

Source:
Green Book, 2nd ed., p. 14
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 970

electric current density, j

A vector quantity the scalar product of which with the cross sectional area vector is equal to the electric current. By magnitude it is the electric current divided by the cross sectional area.

Source:
Green Book, 2nd ed., p. 14
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971

electric dipole moment, p

Vector quantity, the vector product of which with the electric field strength, $\boldsymbol{E}$, of a homogeneous field is equal to the torque. $\boldsymbol{T} = \boldsymbol{p} \times \boldsymbol{E}$. The direction of the dipole moment is from the negative to the positive charge.

Source:
Green Book, 2nd ed., p. 24

electric displacement, D

Product of the permittivity and electric field strength.

Source:
Green Book, 2nd ed., p. 14

electric field (strength), E

Force acting on a charge divided by the charge.

Source:
Green Book, 2nd ed., p. 14
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971

electric mobility, u, μ

Speed of ions divided by the electric field strength in the phase concerned.
See also: mobility

Source:
Green Book, 2nd ed., p. 60
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 982

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971

electric polarizability, α

Tensor quantity relating the induced electric dipole moment, $\boldsymbol{p}_{\mathrm{i}}$, to the applied electric field strength, $\boldsymbol{E}$, $\boldsymbol{p}_{\mathrm{i}} = \alpha \boldsymbol{E}$.

Source:
Green Book, 2nd ed., p. 22

electric potential, V

At a point, the work required to bring a charge from infinity to that point in the electric field divided by the charge.

Source:
Green Book, 2nd ed., p. 14
ISO 31-4: 1992

electric potential difference, ΔV

of a galvanic cell

Difference in the potentials of electrodes on the right and left of a galvanic cell. When ΔV is positive, positive charge flows from left to right through the cell.
Note:
The limiting value of E_{cell} for zero current flowing through the cell, all local charge transfer and chemical equilibria being established, was formerly called emf (electromotive force). The name electromotive force and the symbol emf are no longer recommended, since a potential difference is not a force.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971
Green Book, 3rd ed., p. 71

electric resistance, R

1. To direct current, the potential difference divided by the current when there is no electromotive force in the conductor.
2. To alternating current, the real part of impedance.

Source:
Green Book, 2nd ed., p. 15
ISO 31-4: 1992
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971

electric resistivity

See: resistivity

Source:
Green Book, 2nd ed., p. 15
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971

electric sector

in mass spectrometry

An arrangement of two conducting sheets forming a capactor and giving a radial electrostatic field which is used to deflect and focus ion beams of different energies. The capacitor may, for example, be cylindrical, spherical or toroidal.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1544

electrical arc

A self-sustaining electrical discharge between at least two electrodes, characterized by a comparatively small cathode fall voltage, a low burning voltage and a relatively high current density. The burning voltage of an arc is the voltage across the electrode gap during an arc discharge.

Source:
Orange Book, p. 123

electrical hygrometer

A hygrometer whose sensitive element has electrical properties which vary with the humidity of the gas which traverses the hygrometer.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

electrically conducting polymer

Polymeric material that exhibits bulk electric conductivity.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2070

electrified interphase

An interphase between phases containing free charged components which are usually accumulated or depleted in the surface region thus giving rise to net charges on the phase. This definition includes the special case when the net charge on each of the phases reduces to zero. Charged components may or may not cross the interface between two phases, so that interphases may be divided into the limiting types unpolarizable and polarizable, respectively. Ideally unpolarizable interphases are those for which the exchange of common charged particles between the phases proceeds unhindered. Ideally polarizable interphases are those for which there are no common components between the phases or the exchange of these is hindered. This condition may arise as a result of the equilibrium conditions or from the kinetics of charge transfer and leads to an interphase which is impermeable to electric charge. Real interphases may approach more or less well one of these idealized cases. Polarisibility or non-polarisibility is not an absolute property of an interphase but depends on a number of conditions, e.g. time scale of the experiment.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

electro-dialysis

Membrane-based separation process in which ions are driven through an ion-selective membrane under the influence of an electric field.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1488
This definition supersedes an earlier definition of electrodialysis.

electro-endosmosis

See: electro-osmosis

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

electro-osmosis

Process in which water is transported across the thickness of an anion- exchange or cation-exchange membrane under an applied electric field.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1488
This definition supersedes an earlier definition of electro-osmosis.

electro-osmotic hold-up time, t_{eo}

in capillary electromigration

Time required for a liquid in a capillary to move due to electro-osmosis through the effective length of the capillary, L_{eff}. This time is usually measured as the migration time of a neutral compound, called an electro-osmotic flow marker which is assumed to have an electro-osmotic mobility that is negligible compared to that of the analyte.

Source:
PAC, 2004, *76*, 443 *(Terminology for analytical capillary electromigration techniques (IUPAC Recommendations 2003))* on page 447

electro-osmotic mobility, u or μ_{eo}

in capillary electromigration

Electro-osmotic velocity divided by electric field (strength)

$$\mu_{eo} = \frac{\nu_{eo}}{E}$$

Source:
PAC, 2004, *76*, 443 *(Terminology for analytical capillary electromigration techniques (IUPAC Recommendations 2003))* on page 447

electro-osmotic pressure

The pressure difference Δp across the membrane, plug, etc., needed just to stop electro-osmotic volume flow. Δp is positive if the higher pressure is on the high potential side.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

electro-osmotic velocity

See: electro-osmosis

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

electro-osmotic volume flow

The volume flow per unit time per unit field strength through the whole plug.
See also: electro-osmosis

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

electroactive substance

In voltammetry and related techniques, a substance that undergoes a change of oxidation state, or the breaking or formation of chemical bonds, in a charge-transfer step. If an electroactive substance **B** is formed, in the solution or electrode, by a chemical reaction from another substance **C**, the substance **C** should be called the precursor of **B**. In potentiometry with ion-selective electrodes, a material containing, or in ion-exchange equilibrium with, the sensed ion. The electroactive substance is often incorporated in an inert matrix such as poly(vinyl chloride) or silicone rubber.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1500

electrocapillarity

The dependence of the interfacial tension on the electrical state of the interphase.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 446

electrocapillary equation

A form of the Gibbs adsorption equation which includes an expression of the phenomenon of electrocapillarity:

$$s\,\mathrm{d}T - \tau\,\mathrm{d}p + \mathrm{d}\gamma + \sigma^{\alpha}\,\mathrm{d}E + \sum \mathit{\Gamma}_j\,\mathrm{d}\mu_j = 0$$

where s is the surface excess of entropy of unit area of interphase, T is the temperature, τ is the thickness or excess volume of unit area of the interphase, p is the external pressure, γ is the interfacial tension, σ^{α} is the free surface charge density on phase α (areal amount of charge on the surface of phase α), E is the generalized potential, $\mathit{\Gamma}_j$ is the surface excess, μ_j is the chemical potential and j is an electrically neutral component of one or other of the phases; the sum is over all the components but one in each phase.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 446

electrochemical detector

in gas chromatography

An electrochemical cell which responds to certain substances in the carrier gas eluting from the column. The electrochemical process may be an oxidation, reduction or a change in conductivity.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

electrochemical method of detection

in analysis

A method in which either current or potential is measured during an electrochemical reaction. The gas or liquid containing the trace impurity to be analysed is sent through an electrochemical cell containing a liquid or solid electrolyte and in which an electrochemical reaction specific to the impurity takes place.
See also: amperometric detection method, coulometric detection method, potentiometric detection method

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

electrochemical potential

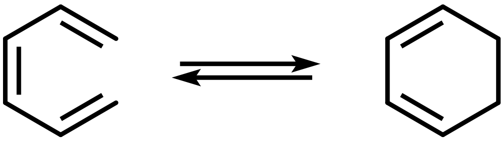
Of a substance in a specified phase, the partial molar Gibbs energy of the substance at the specified electric potential.

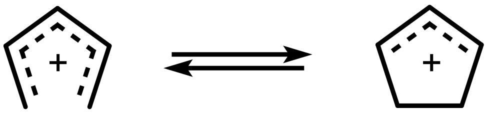
Source:
Green Book, 2nd ed., p. 59

electrocyclic reaction

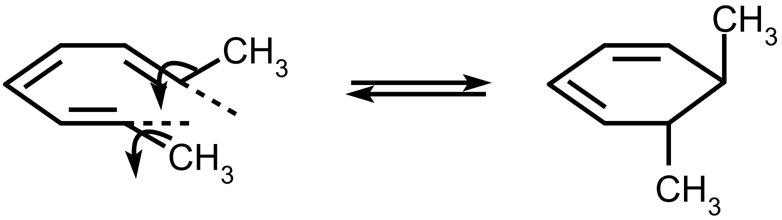
Also contains definitions of: conrotatory, disrotatory

A molecular rearrangement that involves the formation of a σ-bond between the termini of a fully conjugated linear π-electron system (or a linear fragment of a π-electron system) and a decrease by one in the number of π-bonds, or the reverse of that process. For example:

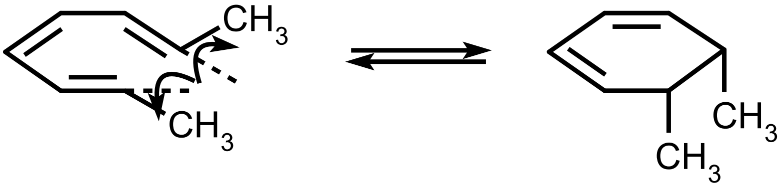




The stereochemistry of such a process is termed 'conrotatory' or antarafacial if the substituents at the interacting termini of the conjugated system both rotate in the same sense, e.g.



or 'disrotatory' (or suprafacial) if one terminus rotates in a clockwise and the other in a counter-clockwise sense, e.g.



See also: pericyclic reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1108

electrode current density, *j*

If the charging current is negligible, in the case of a single electrode reaction, the electrode current density (c.d.) of the electric current flowing through the electrode is related to the flux density of a species **B** by the equation:

$$j = n\,\nu_{\mathrm{B}}{}^{-1}\,F\,(N_{\mathrm{B}})_e$$

where $(N_{\mathrm{B}})_e$ is the normal component of the vector N_{B} at the electrode-solution interface, n is the charge number of the electrode reaction and ν_{B} is the stoichiometric number of species **B**. The ratio $\frac{n}{\nu_{\mathrm{B}}}$ is to be taken as positive if the species **B** is consumed in a cathodic reaction or produced in an anodic reaction. Otherwise it is to be taken as negative. With the convention that the normal distance vector points into the electrolytic solution, a cathodic current is then negative, an anodic current positive.

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1835

electrode potential, E

Electromotive force of a cell in which the electrode on the left is a standard hydrogen electrode and the electrode on the right is the electrode in question.

Source:
Green Book, 2nd ed., p. 61
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971

electrode process

The totality of changes occurring at or near a single electrode during the passage of current.

Source:
PAC, 1980, *52*, 233 *(Electrode reaction orders, transfer coefficients and rate constants. Amplification of definitions and recommendations for publication of parameters)* on page 235

electrode reaction

For an electrode process at a given potential the current is controlled by the kinetics of a number of steps which include the transport of reactants to and from the interface and the interfacial reaction itself. The latter, which is called the electrode reaction, must always include at least one elementary step in which charge is transferred from one phase to the other, but may also involve purely chemical steps within the interfacial region.

Source:
PAC, 1980, *52*, 233 *(Electrode reaction orders, transfer coefficients and rate constants. Amplification of definitions and recommendations for publication of parameters)* on page 235

electrode reaction rate constants

Also contains definitions of: conditional rate constant of an electrode reaction, standard rate constant of an electrode reaction

The electrode reaction rate constants are related to the partial currents by

$$k_{\mathrm{ox}} = \frac{I_{\mathrm{a}}}{n\,F\,A\;\Pi\,c_i^{\nu_i}}$$

$$k_{\mathrm{red}} = \frac{I_{\mathrm{c}}}{n\,F\,A\;\Pi\,c_i^{\nu_i}}$$

where k_{ox} and k_{red} are the rate constants for the oxidizing (anodic) and reducing (cathodic) reactions respectively, n is the charge number of the cell reaction, F is the Faraday constant and A is the geometric area of the electrode, the product $\Pi\, c_i^{\nu_i}$ includes all the species i which take part in the partial reaction, c_i is the volume concentration of species i and ν_i is the order of the reaction with respect to species i. The conditional rate constant of an electrode reaction is the value of the electrode reaction rate constant at the conditional (formal) potential of the electrode reaction. When α the transfer coefficient is independent of potential,

$$k_{\mathrm{c}} = \frac{k_{\mathrm{ox}}}{\mathrm{e}^{\frac{\alpha_{\mathrm{a}}\left(E-E_{\mathrm{c}}^{0'}\right) n F}{\nu R T}}} = \frac{k_{\mathrm{red}}}{\mathrm{e}^{\frac{-\alpha_{\mathrm{c}}\left(E-E_{\mathrm{c}}^{0'}\right) n F}{\nu R T}}}$$

where α_{a} and α_{c} are the anodic and cathodic transfer coefficients respectively, E is the electric potential difference, E_{c} is the conditional (formal) potential, ν is the stoichiometric number, R is the gas constant and T is the thermodynamic temperature. Similar rate constants can be defined using activities in place of concentrations in the first two equations, and the standard electrode potential in place of the conditional potential in the latter two equations. This type of rate constant is called the standard rate constant of the electrode reaction. The observable electrode rate constant is the constant of proportionality expressing the dependence of the rate of the electrode reaction on the interfacial concentration of the chemical species involved in the reaction.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 515
PAC, 1980, *52*, 233 *(Electrode reaction orders, transfer coefficients and rate constants. Amplification of definitions and recommendations for publication of parameters)* on page 236

electrodecantation (or electrophoresis convection)

Electrodialysis may lead to local differences in concentration and density. Under the influence of gravity these density differences lead to large scale separation of sols of high and of low (often vanishingly low) concentrations. This process is called electrodecantation.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 609

electrodeposition

The deposition of dissolved or suspended material by an electric field on an electrode. (Includes electro-crystallization).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

electrofuge

A leaving group that does not carry away the bonding electron pair. For example, in the nitration of benzene by NO_2^+, H^+ is the electrofuge. The adjective of electrofuge is electrofugal.
See also: electrophile, nucleofuge

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1109

electrogenerated chemiluminescence (ECL)

Synonyms: electrochemiluminescence, electroluminescence

Luminescence produced by electrode reactions. Also called electroluminescence or electrochemiluminescence.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2238

electrographite

A synthetic graphite made by electrical heating of graphitizable carbon.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 488

electrokinetic potential, ζ

Potential drop across the mobile part of the double layer, that is responsible for electrokinetic phenomena. ζ is positive if the potential increases from the bulk of the liquid phase towards the interface. In calculating the electrokinetic potential from electrokinetic phenomena it is often asumed that the liquid adhering to the solid wall and the mobile liquid are separated by a sharp shear plane. As long as there is no reliable information on the values of the permittivity and the viscosity in the electrical double layer close to the interface, the calculation of the electrokinetic potential from electrokinetic experiments remains open to criticism. It is therefore essential to indicate in all cases which equations have been used in the calculation of ζ. It can be shown, however, that for the same assumptions about the permittivity and viscosity all electrokinetic phenomena must give the same value for the electrokinetic potential.

Source:
Green Book, 2nd ed., p. 60
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971
PAC, 1994, *66*, 891 *(Quantities and units for electrophoresis in the clinical laboratory (IUPAC Recommendations 1994))* on page 894

electroluminescent polymer

Polymeric material that shows luminescence when an electric current passes through it such that charge carriers can combine at luminescent sites to give rise to electronically excited states of luminescent groups or molecules.

Notes:

1. Electroluminescent polymers are often made by incorporating luminescent groups or dyes into conducting polymers.
2. Electrogenerated chemiluminescence directly connected with electrode reactions may also be called electroluminescence.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 899

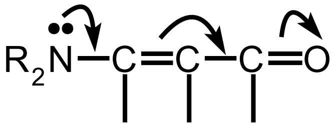
electrolytic hygrometer

Hygrometer using a hygroscopic substance (for example, diphosphorus pentaoxide, P_2O_5) which is transformed into an electrolyte (phosphoric acid, H_3PO_4) in contact with the moisture in the gas. The electrolyte (phosphoric acid) is electrolysed continuously and the electrolysis current is measured. At a constant flow of the gas to be analysed, the electrolysis current is a linear function of the water concentration.

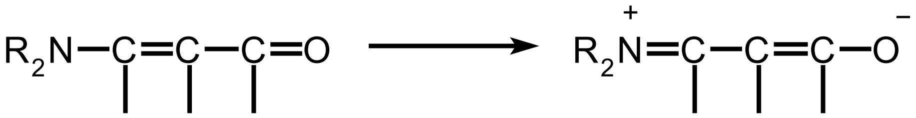
Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

electromeric effect

A molecular polarizability effect occurring by an intramolecular electron displacement (sometimes called the 'conjugative mechanism' and, previously, the 'tautomeric mechanism') characterized by the substitution of one electron pair for another within the same atomic octet of electrons. It can be indicated by curved arrows symbolizing the displacement of electron pairs, as in:



which represents the hypothetical electron shift



$$R_2N{-}C{=}C{-}C{=}O \longrightarrow R_2\overset{+}{N}{=}C{-}C{=}C{-}\overset{-}{O}$$

The term has been deemed obsolescent or even obsolete (see mesomeric effect, resonance effect). It has long been custom to use phrases such as 'enhanced substituent resonance effect' which imply the operation of the electromeric effect, without using the term, and various modern theoretical treatments parametrize the response of substituents to 'electronic demand', which amounts to considering the electromeric effect together with the inductomeric effect.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1109

electromigration

The transport of particles under the influence of an electric field.

Source:
PAC, 1999, *71*, 1307 *(Definitions of Terms for Diffusion in the Solid State)* on page 1314

electromotive force, E

Energy supplied by a source divided by the electric charge transported through the source. For a galvanic cell it is equal to the electric potential difference for zero current through the cell.

Source:
Green Book, 2nd ed., p. 58
ISO 31-4: 1992
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971

electron

Elementary particle not affected by the strong force having a spin quantum number $\frac{1}{2}$, a negative elementary charge and a rest mass of $0.000\ 548\ 579\ 903(13)\ \mathrm{u}$.

Source:
Green Book, 2nd ed., p. 93

See also:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1540

electron acceptor

1. A substance to which an electron may be transferred; for example 1,4-dinitrobenzene or the dication 1,1'-dimethyl-4,4'-bipyridyldiium.
2. [obsolete] A Lewis acid. This usage is discouraged.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1109

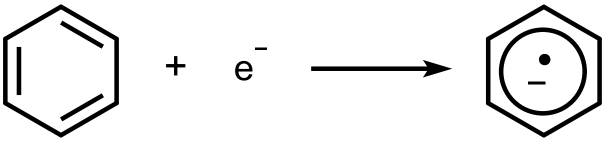
electron affinity, E_{ea}

Energy required to detach an electron from the singly charged negative ion (energy for the process $X^{-} \longrightarrow X + e$). The equivalent more common definition is the energy released ($E_{\text{inititial}} - E_{\text{final}}$) when an additional electron is attached to a neutral atom or molecule.

Source:
Green Book, 2nd ed., p. 20
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1109
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

electron attachment

The transfer of an electron to a molecular entity, resulting in a molecular entity of (algebraically) increased negative charge. It is not an attachment.



See also: oxidation (1), reduction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1109
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

electron back-transfer

Thermal inversion of excited-state electron transfer restoring the donor and acceptor in their original oxidation state. In using this term one should also specify the resulting electronic state of the donor and acceptor. This term is preferred to back electron-transfer.
Notes:

1. It is recommended to use this term only for the process restoring the original electronic state of donor and acceptor.
2. Should the forward electron transfer lead to charge separation, electron back-transfer will result in charge recombination.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 329

electron beam curing

Also contains definition of: EB curing

Curing induced by electron beam irradiation.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1822

electron capture

A nuclear transformation in which the nucleus captures an orbital electron. Often the shell, from which the electron is captured, is indicated. (K-, L-, etc.).

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

electron capture detector

in gas chromatography

A small radioactive source containing ^{3}H or ^{63}Ni ionizes the molecules of the carrier gas (nitrogen or argon–methane), and a potential difference creates a small current. This current is reduced when an electronegative substance (such as a halocarbon) is introduced. The reduction in current is a measure of the concentration of the electronegative substance. The detection limit (threshold) varies greatly according to the substances to be analysed and can reach a mixing ratio of 10^{-12}. The linear dynamic range may be 10^{4} but the maximum measuring value generally lies below $1\ \mathrm{ppmv}$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

electron charge

The negative electric charge which appears on the electron or univalent ions [1.602×10^{-19} coulombs or 4.803×10^{-10} electrostatic units (esu)].

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

electron correlation

The adjustment of electron motion to the instantaneous (as opposed to time-averaged) positions of all the electrons in a molecular entity.
See also: correlation energy

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2238

electron density

If $P(x, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$ is the probability of finding an electron in the volume element $\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$ at the point of a molecular entity with coordinates x, y, z, then $P(x, y, z)$ is the electron density at this point. For many purposes (e.g. X-ray scattering, forces on atoms) the system behaves exactly as if the electrons were spread out into a continuously distributed charge. The term has frequently been wrongly applied to negative charge population.
See also: charge density

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1110

electron density function

The electron probability distribution function, ρ, defined as

$$\rho(\mathbf{r}) = n \int \Psi^{*}[\mathbf{r}(1),\ \mathbf{r}(2) \ldots \mathbf{r}(n)]\ \Psi[\mathbf{r}(1),\ \mathbf{r}(2) \ldots \mathbf{r}(n)]\mathrm{d}\mathbf{r}(2) \ldots \mathrm{d}\mathbf{r}(n)$$

where Ψ is an electronic wave-function and integration is made over the coordinates of all but the first electron of n. The physical interpretation of the electron density function is that $\rho\ \mathrm{d}\mathbf{r}$ gives the probability of finding an electron in a volume element $\mathrm{d}\mathbf{r}$, *i.e.*, electron density in this volume.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1937

electron detachment

The reverse of an electron attachment.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1110

electron donor

1. A molecular entity that can transfer an electron to another molecular entity, or to the corresponding chemical species.
2. [obsolete] A Lewis base. This use is discouraged.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1110

electron energy

in mass spectrometry

The potential difference through which electrons are accelerated before they are used to bring about electron ionization.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

electron exchange excitation transfer

Synonymous with Dexter excitation transfer.
See also: energy transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2238

electron impact ionization [obsolete]

in mass spectrometry

See: electron ionization

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

electron ionization

in mass spectrometry

This is the term used to describe ionization of any species by electrons. The process may, for example, be written:

- for atoms or molecules:

$$\mathrm{M} + \mathrm{e} \rightarrow \mathrm{M}^{+\bullet} + 2\,\mathrm{e}$$

- for radicals:

$$\mathrm{M}^{\bullet} + \mathrm{e} \rightarrow \mathrm{M}^{+} + 2\,\mathrm{e}$$

The term 'electron impact' should not be used.
See: radical ion for a note concerning the symbolic representation of radical ions;
See also: photoionization

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

electron jump

The term can be applied to a reaction in which there is an electron transfer with the formation of an ionic intermediate.

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 767

electron kinetic energy

The difference between the energy of the exciting photon and the ionization energy.

Source:
PAC, 1976, *45*, 221 *(Nomenclature and Spectral Presentation in Electron Spectroscopy Resulting from Excitation by Photons)* on page 223

electron microscopy

See: transmission electron microscopy (TEM)

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2024

electron paramagnetic resonance (EPR)

Electron paramagnetic resonance (EPR) and/or electron spin resonance (ESR) is defined as the form of spectroscopy concerned with microwave-induced transitions between magnetic energy levels of electrons having a net spin and orbital angular momentum. The term electron paramagnetic resonance and the symbol EPR are preferred and should be used for primary indexing.

Source:
PAC, 1989, *61*, 2195 *(Recommendation for EPR/ESR nomenclature and conventions for presenting experimental data in publications (Recommendations 1989))* on page 2196

electron probe microanalysis (EPMA)

General term for methods using bombardment of a solid specimen by electrons which generate a variety of signals providing the basis for a number of different analytical techniques.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2024

electron probe X-ray microanalysis (EPXMA)

Any analytical technique which uses the excitation and evaluation of the characteristic X-ray spectrum of a solid specimen by a focused electron beam (typically of a diameter of less than

1 μm). Qualitative and quantitative X-ray analysis is the main feature of EPXMA. For obtaining supplementary information the secondary, back scattered and absorbed electrons are also frequently observed. Qualitative and quantitative X-ray analysis is, however, the main feature of EPXMA.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2024

electron rest mass

Atomic fundamental physical constant used as atomic unit of mass, $m_{\mathrm{e}} = 9.109\,3897\,(54) \times 10^{-31}$ kg.

Source:
CODATA Bull. 1986, *63*, 1

electron spectroscopy for chemical analysis (ESCA)

Type of spectroscopy involving the measurement of the kinetic energy of electrons emitted by chemical substances usually as a result of excitation by monochromatic X-rays.

Source:
PAC, 1976, *45*, 221 *(Nomenclature and Spectral Presentation in Electron Spectroscopy Resulting from Excitation by Photons)* on page 223

electron stopping power

in X-ray emission spectroscopy

When a beam of electrons strikes a target or specimen there are three ways in which the electrons may lose energy (low energy collisions, X-ray production, and formation of a spectral continuum). The average energy loss per unit distance travelled along the electron path is called electron stopping power, $\frac{\mathrm{d}E}{\mathrm{d}x}$.

Source:
PAC, 1980, *52*, 2541 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - IV X-ray emission spectroscopy)* on page 2545

electron transfer

The transfer of an electron from one molecular entity to another, or between two localized sites in the same molecular entity.
See also: inner sphere (electron transfer), outer sphere (electron transfer), Marcus equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1110

PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2239

electron transfer photosensitization

Photochemical process in which a reaction of a non-absorbing substrate is induced by electron transfer (not energy transfer) with an excited light-absorbing sensitizer. The overall process must be such that the sensitizer is recycled. Depending on the action of the excited sensitizer as electron donor or acceptor the sensitization is called reductive or oxidative.
See also: photosensitization

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2239

electron work function, Φ

The minimum work needed to extract electrons from the Fermi level of a metal M across a surface carrying no net charge. It is equal to the sum of the potential energy and the kinetic Fermi energy taken with the reverse sign:

$$\Phi^{M} = -\left(V_{\mathrm{e}} + \varepsilon_{\mathrm{e}}^{F}\right)$$

whera V_{e} is the potential energy for electrons in metals and $\varepsilon_{\mathrm{e}}^{\mathrm{F}}$ is the kinetic energy of electrons at the Fermi level.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 441

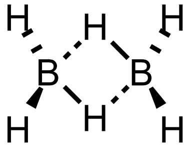
electron-counting rules

Rules establishing correspondence between the topology of a molecular structure and the number of electrons which may be placed into its bonding molecular orbitals. In the origin of various electron-counting rules lies a general assumption that the completeness of the valence electron shell of a molecular entity belonging to a certain structural type serves as the major criterion of structural stability.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1936

electron-deficient bond

A single bond between adjacent atoms that is formed by less than two electrons, as in B_2H_6:



The B–H–B bonds are called a 'two-electron three-centre bonds'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1110

electron-deficient compounds

Molecules or ions that contain too few electrons to allow their bonding to be described exclusively in terms of two-center, two-electron, *i.e.,* covalent, bonds. Such molecules or certain fragments in these are often held together by the multicenter bonds.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1936

electron-donor-acceptor complex [obsolete]

A term sometimes employed instead of charge-transfer complex or Lewis adduct.
See also: adduct, coordination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1110

electron-pair acceptor

A synonym for Lewis acid.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1110

electron-pair donor

A synonym for Lewis base.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1110

electron-transfer catalysis

The term indicates a sequence of reactions such as shown in equations (1)–(3), leading from A to B :

$$\mathrm{A} + \mathrm{e}^{-} \rightarrow \mathrm{A}^{\bullet -} \quad (1)$$

$$\mathrm{A}^{\bullet -} \rightarrow \mathrm{B}^{\bullet -} \quad (2)$$

$$\mathrm{B}^{\bullet -} + \mathrm{A} \rightarrow \mathrm{B} + \mathrm{A}^{\bullet -} \quad (3)$$

An analogous sequence involving radical cations ($\mathrm{A}^{+\cdot}$, $\mathrm{B}^{+\cdot}$) is also observed. The most notable example of electron-transfer catalysis is the $\mathrm{S_{RN}1}$ (or $\mathrm{T} + \mathrm{D_N} + \mathrm{A_N}$) reaction of aromatic halides. The term has its origin in a suggested analogy to acid-base catalysis, with the electron instead of the proton. However, there is a difference between the two catalytic mechanisms, since the electron is not a true catalyst, but rather behaves as the initiator of a chain reaction. 'Electron-transfer induced chain reaction' is a more appropriate term for the situation described by equations (1)–(3).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1110

electronation

See: electron attachment, reduction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1111

electronegativity

Concept introduced by L. Pauling as the power of an atom to attract electrons to itself. There are several definitions of this quantity. According to Mulliken it is the average of the ionization energy and electron affinity of an atom, but more frequently a relative scale due to Pauling is used where dimensionless relative electronegativity differences are defined on the basis of bond dissociation energies, E_{d}, expressed in electronvolts:

$$\chi_{\mathrm{r}}(\mathrm{A}) - \chi_{\mathrm{r}}(\mathrm{B}) = (\mathrm{eV})^{-1/2} \sqrt{E_{\mathrm{d}}(\mathrm{AB}) - \frac{1}{2}\left[E_{\mathrm{d}}(\mathrm{AA}) + E_{\mathrm{d}}(\mathrm{BB})\right]}$$

The scale is chosen so as to make the relative electronegativity of hydrogen $\chi_{\mathrm{r}} = 2.1$. The sign of the square root was chosen intuitively by Pauling.

Source:
Green Book, 2nd ed., p. 20
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1111

electroneutrality principle

The principle expresses the fact that all pure substances carry a net charge of zero.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1111

electronic chemical potential

The quantity that measures the escaping tendency of electrons from a species in its ground state. It is the negative of the absolute electronegativity.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1937

electronic effect of substituents: symbols and signs

The inductive effect has universally been represented by the symbol I. This is now commonly taken to include both through-bonds and through-space transmission, but I is also used specifically for through-bonds transmission; through-space transmission is then symbolized as F (for field effect). The symbols for the influence of substituents exerted through electron delocalization have variously been M (mesomeric), E (electromeric), T (tautomeric), C (conjugative), K (konjugativ) and R (resonance). Since the present fashion is to use the term resonance effect, R is the most commonly used symbol, although M is still seen quite often. Both the possible sign conventions are in use. The Ingold sign convention associates electronegativity (relative to hydrogen atom) with a negative sign, electropositivity with a positive sign. Thus the nitro group is described as electronwithdrawing by virtue of its $-\mathrm{I}$ and $-\mathrm{M}$ effects; chloro is described as a $-\mathrm{I}, +\mathrm{M}$ substituent, etc. For correlation analysis and linear free-energy relationships this convention has been found inconvenient, for it is in contradiction to the sign convention for polar substituent constants (σ-constants). Authors concerned with these fields often avoid this contradiction by adopting the opposite sign convention originally associated with Robinson, for electronic effects. This practice is almost always associated with the use of R for the electron delocalization effect: thus the nitro group is a $+\mathrm{I}, +\mathrm{R}$ substituent; chloro a $+\mathrm{I}, -\mathrm{R}$ substituent, etc.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1111

electronic energy migration (or hopping)

The movement of electronic excitation energy from one molecular entity to another of the same species, or from one part of a molecular entity to another of the same kind (e.g. excitation migration between the chromophores of an aromatic polymer). The migration can happen via radiative or radiationless processes.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2238

electronic stability

Unavailability of another electronic structure (different electronic state) of lower energy with the same number of electrons.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1938

electronic state

An arrangement allowed by the laws of quantum mechanics of electrons within an atom, molecule (or system of molecules).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1937

electronically excited state

A state of an atom or molecular entity which has greater electronic energy than the ground state of the same entity.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2238

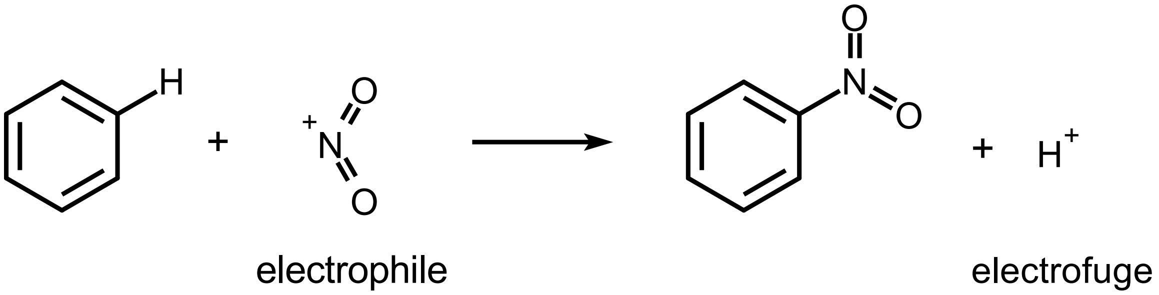
electronvolt

Non-SI unit of energy, $\mathrm{eV} \approx 1.602\ 176\ 487(40) \times 10^{-19}\ \mathrm{J}$.

Source:
CODATA 2006
Green Book, 2nd ed., p. 75
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 971

electrophile (electrophilic)

An electrophile (or electrophilic reagent) is a reagent that forms a *bond* to its reaction partner (the nucleophile) by accepting both bonding electrons from that reaction partner. An 'electrophilic substitution reaction ' is a heterolytic reaction in which the reagent supplying the entering group acts as an electrophile. For example:



Electrophilic reagents are Lewis acids. 'Electrophilic catalysis' is catalysis by Lewis acids. The term 'electrophilic' is also used to designate the apparent polar character of certain radicals as inferred from their higher relative reactivities with reaction sites of higher electron density.
See also: electrophilicity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1111

electrophilicity

1. The property of being electrophilic (see electrophile).
2. The relative reactivity of an electrophilic reagent. (It is also sometimes referred to as 'electrophilic power'.) Qualitatively, the concept is related to Lewis acidity. However, whereas Lewis acidity is measured by relative equilibrium constants, electrophilicity is measured by relative rate constants for reactions of different electrophilic reagents towards a common substrate (usually involving attack at a carbon atom).
   See also: nucleophilicity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1111

electrophoresis

The motion of colloidal particles in an electric field. The term cataphoresis should be abandoned.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 619

electrophoretic mobility, μ

The observed rate of migration of a component (v) divided by electric field strength (E) in a given medium.
Notes:

1. Mobilities are sometimes expressed with a negative sign, because migration of the solutes or particles generally occurs in the direction opposite to the electrophoretic field (which is taken as reference for that direction).
2. In a solid support medium, only apparent values can be determined.

Source:
PAC, 1994, *66*, 891 *(Quantities and units for electrophoresis in the clinical laboratory (IUPAC Recommendations 1994))* on page 894

electrophoretic velocity, ν_{ep}

The velocity of a charged analyte under the influence of an electric field relative to the background electrolyte. Also called rate of migration (in electrophoresis).

Source:
PAC, 2004, *76*, 443 *(Terminology for analytical capillary electromigration techniques (IUPAC Recommendations 2003))* on page 448

electrophotography

Processes of photoimaging which are based on photo-induced changes of electric fields (photoconductive or photo-electrostatic effects).

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2239

electrosmosis [obsolete]

See: electro-osmosis

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

electrostatic filter

Filters for which an electrostatic charge is applied to the filter element. A fibrous filter material is often pleated in between V-shaped supports consisting of electrostatically charged, metal rods which are insulated from the supporting frame.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

electrostatic precipitator

A device which separates particles from a gas stream by passing the carrier gas between pairs of electrodes across which a unidirectional, high-voltage potential is placed. The particles are charged before passing through the field and migrate to an oppositely charged electrode. These devices are very efficient collectors of small particles, and their use in removing particles from power plant plumes and in other industrial applications is widespread.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

electrostriction

Contraction of a dielectric in an electric-field gradient.
Notes:

1. For example, the contraction taking place around the charged centres created as a consequence of the sudden formation of separated positive and negative charges in the process of *electron transfer*.
2. The thermodynamic description of electrostriction was given by Drude and Nernst in 1894 to explain the phenomenon of contraction of a continuum medium, such as an alkane, around charges suddenly produced in that medium.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 331

electrothermal atomizer

Also contains definitions of: confined atomizer, open atomizer

in spectrochemical analysis

A device which is heated to the temperature required for analyte atomization by the passage of electrical current through its body. In open atomizers the sample vapour, together with analyte atoms, leaving the atomizer surface may move freely into the surrounding space. In confined atomizers the sample vapour is restricted by the atomizer wall except for the openings where the optical beam enters and leaves the atomizer and the sample introduction hole.

Source:
PAC, 1992, *64*, 253 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XII. Terms related to electrothermal atomization (IUPAC Recommendations 1992))* on page 254

electroviscous effects

For dispersions of charged particles, these are those components of the viscosity connected with the charge of the particles.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

element

See: chemical element

Source:
Physical Chemistry Division, unpublished
Red Book, p. 35

element effect

The ratio of the rate constants of two reactions that differ only in the identity of the element of the atom in the leaving group, e.g. $\frac{k_{\mathrm{Br}}}{k_{\mathrm{Cl}}}$. As for isotope effects, a ratio of unity is regarded as a 'null effect'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1111

elementary charge

Also contains definition of: proton charge

Electromagnetic fundamental physical constant equal to the charge of a proton and used as atomic unit of charge $e = 1.602\ 176\ 487\ \ (40) \times 10^{-19}\ \mathrm{C}$.
See also: electric charge

Source:
CODATA 2006
Green Book, 2nd ed., p. 14
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 972

elementary entity

Any countable object or event, but usually a molecule, an ion or a specified group of atoms.

Source:
Physical Chemistry Division, unpublished

elementary particle

in nuclear chemistry

A particle in which, at the present, no structure can be observed at moderate energies.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

elementary reaction

A reaction for which no reaction intermediates have been detected or need to be postulated in order to describe the chemical reaction on a molecular scale. An elementary reaction is assumed to occur in a single step and to pass through a single transition state.
See also: stepwise reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1111
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2294

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 163

elimination

The reverse of an addition reaction or transformation. In an elimination two groups (called eliminands) are lost most often from two different centres (1/2/elimination or 1/3/elimination, etc.) with concomitant formation of an unsaturation in the molecule (double bond, triple bond) or formation of a new ring. If the groups are lost from a single centre (α-elimination, 1/1/elimination) the resulting product is a carbene or a 'carbene analogue'.
See also: α-elimination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

eluate

The effluent from a chromatographic bed emerging when elution is carried out.

Source:
Orange Book, p. 99

eluent

The liquid or gas entering a chromatographic bed and used to effect a separation by elution.

Source:
Orange Book, p. 97

elute

To chromatograph by elution chromatography. This term is preferred to the term 'develop', which has been used in paper chromatography and in thin-layer chromatography. The process of elution may continue until the components have left the chromatographic bed.

Source:
Orange Book, p. 95
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 824
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

elution

See: selective elution, stepwise elution, gradient elution

Source:
Orange Book, p. 92

elution band

in chromatography

Synonymous with chromatographic peak.

Source:
Orange Book, p. 96
Orange Book, p. 101

elution chromatography

A procedure for chromatographic separation in which the mobile phase is passed through the chromatographic bed after the application of the sample.

Source:
Orange Book, p. 92
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 824

elution curve

A chromatogram or part of a chromatogram recorded when elution techniques are used.

Source:
Orange Book, p. 95

elutriation

The process of separating the lighter particles of a powder from the heavier ones by means of an upward directed stream of fluid (gas or liquid).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

emanation thermal analysis

A thermoanalytical technique in which the release of radioactive emanation from a substance (and/or its reaction product(s)) is measured as a function of temperature whilst the substance is subjected to a controlled temperature programme.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1739

embryo

Also contains definitions of: critical embryo, homogeneous nucleus

An aggregate of a small number of atoms, molecules or ions. An embryo of such a size that the Gibbs energy at constant pressure and temperature is a maximum is called a critical embryo. An embryo larger than a critical embryo is called a homogeneous nucleus. Colloidal sols may be formed by condensation methods. When a condensation method is applied, molecules (or ions) are deposited on nuclei which may be of the same chemical species as the colloid (homogeneous nucleation) or different (heterogeneous nucleation).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

emission

Radiative deactivation of an excited state; transfer of energy from a molecular entity to an electromagnetic field.
See also: fluorescence, luminescence, phosphorescence

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2239

emission anisotropy

Also contains definitions of: degree of (polarization) anisotropy, luminescence anisotropy

Also contains definition of: time-resolved anisotropy, $r(t)$

Used to characterize luminescence (fluorescence, phosporescence) polarization resulting from photoselection. Defined as:

$$r = \frac{I_{\parallel} - I_{\perp}}{I_{\parallel} + 2\, I_{\perp}}$$

where $I_{\parallel}$ and $I_{\perp}$ are the intensities measured with the linear polarizer for emission parallel and perpendicular, respectively, to the electric vector of linearly polarized incident electromagnetic radiation (which is often vertical). The quantity $I_{\parallel} + 2\, I_{\perp}$ is proportional to the total fluorescence intensity I.

Notes:

1. Fluorescence polarization may also be characterized by the polarization ratio, also called the degree of polarization p,

   $$p = \frac{I_{\parallel} - I_{\perp}}{I_{\parallel} + I_{\perp}}$$

   For parallel absorbing and emitting transition moments the (theoretical) values are $(r,\, p) = (2/5,\, 1/2)$; when the transition moments are perpendicular, the values are $(r,\, p) = (-1/5,\, -1/3)$. In many cases, it is preferable to use emission anisotropy because it is additive; the overall contribution of n components r_i, each contributing to the total fluorescence intensity with a fraction $f_i = I_i/I$, is given by:

   $r = \sum_{i=1}^{n} f_i\, r_i$ with $\sum_{i=1}^{n} f_i = 1$
2. On continuous illumination, the measured emission anisotropy is called steady-state emission anisotropy ($\bar{r}$) and is related to the time-resolved anisotropy by:

   $$\bar{r} = \frac{\int_0^{\infty} r(t)\, I(t) \mathrm{d}t}{\int_0^{\infty} I(t) \mathrm{d}t}$$

   where $r(t)$ is the anisotropy and $I(t)$ is the radiant intensity of the emission, both at time t following a δ-pulse excitation.
3. Luminescence polarization spectroscopy, with linear polarizers placed in both beams, is usually performed on isotropic samples, but it may also be performed on oriented anisotropic samples. In the case of an anisotropic, uniaxial sample, five linearly independent luminescence spectra, instead of the two available for an isotropic sample, may be recorded by varying the two polarizer settings relative to each other and to the sample axis.

4. The term fundamental emission anisotropy describes a situation in which no depolarizing events occur subsequent to the initial formation of the emitting state, such as those caused by rotational diffusion or energy transfer. It also assumes that there is no overlap between differently polarized transitions. The (theoretical) value of the fundamental emission anisotropy, r_0, depends on the angle α between the absorption and emission transition moments in the following way:

$$r_0 = < 3\cos^2\alpha - 1 > / 5$$

   where $< \ >$ denotes an average over the orientations of the photoselected molecules. r_0 can take on values ranging from $-1/5$ for $\alpha = 90\,°$ (perpendicular transition moments) to $2/5$ for $\alpha = 0\,°$ (parallel transition moments). In spite of the severe assumptions, the expression is frequently used to determine relative transition-moment angles.
5. In time-resolved fluorescence with δ-pulse excitation, the theoretical value at time zero is identified with the fundamental emission anisotropy.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 332

emission control equipment

in atmospheric chemistry

Air pollution control equipment which either converts the pollutant chemically to a non-polluting substance or collects the pollutant by some means including gravity settling chambers, inertial separators, cyclonic separators, filters, electrical precipitators, scrubbers, (spray towers, jet scrubbers, Venturi scrubbers, inertial scrubbers, mechanical scrubbers and packed scrubbers). Certain gases and odoriferous compounds are controlled by combustion, absorption (spray chambers, mechanical contactors, bubble cap or sieve plate contactors and packed towers) and adsorption units (packed beds or fluidized beds).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2187

emission flux

in atmospheric chemistry

The emission per unit area of the appropriate surface of an emitting source.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2187

emission

in atmospheric chemistry

The total rate at which a solid, liquid or gaseous pollutant is emitted into the atmosphere from a given source; usually expressed as mass per unit time. Primary emissions are those substances which are emitted directly to the atmosphere (e.g. NO, SO_2, etc.), while secondary emissions are formed from the primary emissions through thermal or photochemical reactions (e.g. ozone, aldehydes, ketones, sulfuric acid, nitric acid, etc.). The point or area from which the discharge takes place is called the source; the area in which the emission or its transformed products (e.g. in the case of aerosols, acidic deposition, etc.) may be deposited is called the receptor area or sink. Emission may be applied to noise, heat, etc., as well as pollutants.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

emission spectrum

Plot of the emitted spectral radiant power (spectral radiant exitance) or of the emitted spectral photon irradiance (spectral photon exitance) against a quantity related to photon energy, such as frequency, ν, wavenumber, σ, or wavelength, λ. When corrected for wavelength-dependent variations in the equipment response, it is called a corrected emission spectrum.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2239

See also:
Orange Book, p. 196

emittance, ε

Ratio of radiant exitance of a thermal radiator to that of a full radiator (black body) at the same temperature. In ISO this quantity is called emissivity.

Source:
Green Book, 2nd ed., p. 31
ISO 31-5: 1992 *(Quantities and Units - Part 5: Electricity and Magnetism.)*
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2239
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 972

empirical formula

Formed by juxtaposition of the atomic symbols with their appropriate subscripts to give the simplest possible formula expressing the composition of a compound.

Source:
Red Book, p. 45

emulsifier

A surfactant which when present in small amounts facilitates the formation of an emulsion, or enhances its colloidal stability by decreasing either or both of the rates of aggregation and coalescence.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

emulsion

A fluid colloidal system in which liquid droplets and/or liquid crystals are dispersed in a liquid. The droplets often exceed the usual limits for colloids in size. An emulsion is denoted by the symbol O/W if the continuous phase is an aqueous solution and by W/O if the continuous phase is an organic liquid (an 'oil'). More complicated emulsions such as O/W/O (i.e. oil droplets contained within aqueous droplets dispersed in a continuous oil phase) are also possible. Photographic emulsions, although colloidal systems, are not emulsions in the sense of this nomenclature.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 606

enamines

Alkenylamines; by usage the term refers specifically to vinylic amines, which have the structure $R_2NCR=CR_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1333

enantiomer

One of a pair of molecular entities which are mirror images of each other and non-superposable.
See also: enantiomorph

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

enantiomer excess (enantiomeric excess)

Also contains definition of: percent enantiomer excess

For a mixture of (+)- and (−)-enantiomers, with composition given as the mole or weight fractions $F_{(+)}$ and $F_{(-)}$ (where $F_{(+)} + F_{(-)} = 1$) the enantiomer excess is defined as $\mid F_{(+)} - F_{(-)} \mid$ (and the percent enantiomer excess by $100 \ \mid F_{(+)} - F_{(-)} \mid$). Frequently this term is abbreviated as e.e.

See: optical purity

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

enantiomeric groups

Chiral groups that are mirror images of one another.

Source:
Blue Book, p. 480

enantiomeric purity

See: enantiomer excess

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

enantiomeric ratio

The ratio of the percentage of one enantiomer in a mixture to that of the other e.g. $70(+) : 30(-)$.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

enantiomeric units

in a polymer

Two configurational units that correspond to the same constitutional unit are considered to be enantiomeric if they are non-superposable mirror images.

Source:
Purple Book, p. 27

enantiomerically enriched (enantioenriched)

A sample of a chiral substance whose enantiomeric ratio is greater than $50 : 50$ but less than $100 : 0$.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

enantiomerically pure (enantiopure)

A sample all of whose molecules have (within limits of detection) the same chirality sense. Use of homochiral as a synonym is strongly discouraged.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

enantiomerism

The isomerism of enantiomers.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

enantiomerization

The interconversion of enantiomers.
See: racemization

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

enantiomorph

One of a pair of chiral objects or models that are non- superposable mirror images of each other. The adjective enantiomorphic is also applied to mirror-image related groups within a molecular entity.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

enantioselectivity

See: stereoselectivity

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

enantiotopic

Constitutionally identical atoms or groups in molecules which are related by symmetry elements of the second kind only (mirror plane, inversion centre or rotation–reflection axis). For example the two groups **c** in a grouping **Cabcc** are enantiotopic. Replacement of one of a pair of enantiotopic groups forms one of a pair of enantiomers. Analogously, if complexation or addition to one of the two faces defined by a double bond or other molecular plane gives rise to a chiral species, the two faces are called enantiotopic.
See also: prochiral, diastereotopic

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

enantiotropic mesophase

A mesophase that is thermodynamically stable over a definite temperature or pressure range.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 495

enantiotropic transition

See: polymorphic transition
Note:
In liquid crystal systems this term refers to a liquid crystal to liquid crystal transition that occurs above the melting point.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 581

encapsulation

Also contains definitions of: immobilization by adsorption *in catalysis*, immobilization by inclusion *in catalysis*, reticulation *in catalysis*

in catalysis

Enzymes or cells which are of relatively large size may be entrapped in a maze of polymeric molecules (a gel). This procedure is called immobilization by inclusion. When the biocatalyst is enclosed inside a semipermeable membrane, usually approximately spherical, the method is known as encapsulation. In the process of reticulation the primary biocatalyst particles (individual enzyme molecules, cofactors or individual cells) are covalently attached to each other by organic chains, into a three-dimensional network. The term grafting is also used in this context. Attachment to the support by adsorption forces is called immobilization by adsorption.

Source:
PAC, 1991, *63*, 1227 *(Manual on catalyst characterization (Recommendations 1991))* on page 1230

encounter

A set of collisions between reactant molecules in solids, liquids or dense gases, occurring in rapid succession as a result of the cage effect.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 163

encounter complex

A complex of molecular entities produced at an encounter-controlled rate, and which occurs as an intermediate in a reaction mechanism. When the complex is formed from two molecular entities it is called an 'encounter pair'. A distinction between encounter pairs and (larger) encounter complexes may be relevant in some cases, e.g. for mechanisms involving pre-association.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2239

encounter pair

See: encounter complex

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2239

encounter-controlled rate

A rate of reaction corresponding to the rate of encounter of the reacting molecular entities. This is also known as 'diffusion-controlled rate' since rates of encounter are themselves controlled by diffusion rates (which in turn depend on the viscosity of the medium and the dimensions of the reactant molecular entities). For a bimolecular reaction between solutes in water at $25\ °\mathrm{C}$ an encounter-controlled rate is calculated to have a second-order rate constant of about $10^{10}\ \mathrm{dm^3\ mol^{-1}\ s^{-1}}$.
See also: microscopic diffusion control

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

end-group

A constitutional unit that is an extremity of a macromolecule or oligomer molecule. An end-group is attached to only one constitutional unit of a macromolecule or oligomer molecule.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2294

end-point

See: titration

Source:
Orange Book, p. 47

end-to-end distance

in polymers

The length, r, of the end-to-end vector.

Source:
Purple Book, p. 49

end-to-end vector

in polymers

The vector, $\boldsymbol{r}$, connecting the two ends of a linear polymer chain in a particular conformation.

Source:
Purple Book, p. 49

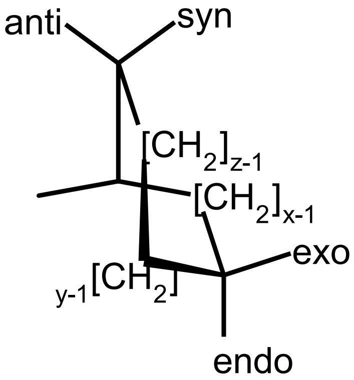
endergonic (or endoergic) reaction

This is usually taken to be a reaction for which the overall standard Gibbs energy change ΔG° is positive. Some workers use this term with respect to a positive value of ΔH° at the absolute zero of temperature.

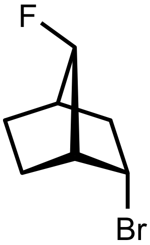
Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 164

endo, *exo*, *syn*, *anti*

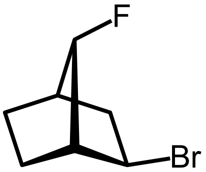
Descriptors of the relative orientation of groups attached to non-bridgehead atoms in a bicyclo[$x.y.z$]alkane ($x \geq y > z > 0$).



If the group is orientated towards the highest numbered bridge (*z* bridge, e.g. C-7 in example below) it is given the description *exo*; if it is orientated away from the highest numbered bridge it is given the description *endo*. If the group is attached to the highest numbered bridge and is orientated towards the lowest numbered bridge (*x* bridge, e.g. C-2 in example below) it is given the description *syn*; if the group is orientated away from the lowest numbered bridge it is given the description *anti*.



2-*endo*-bromo-7-*anti*-fluoro-bicyclo[2.2.1]heptane



2-*exo*-bromo-7-*syn*-fluoro-bicyclo[2.2.1]heptane

See also: *syn*, *anti*

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2207

endocytosis

Uptake of material into a cell by invagination of the plasma membrane and its internalisation in a membrane-bounded vesicle.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1050

endoenzymes

Enzymes that cut internal bonds of a polymer. Endonucleases are able to cleave phosphodiester bonds within a nucleic acid chain by hydrolysis either randomly or at specific base sequences (cf. restriction enzymes).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 152

endothermic reaction

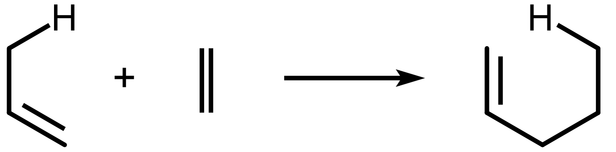
A reaction for which the overall standard enthalpy change ΔH° is positive.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 164

ene reaction

Also contains definitions of: enophile, retro-ene reaction

The addition of a compound with a double bond having an allylic hydrogen (the 'ene') to a compound with a multiple bond (the 'enophile') with transfer of the allylic hydrogen and a concomitant reorganization of the bonding, as illustrated below for propene (the 'ene') and ethene (the 'enophile'). The reverse is a 'retro-ene' reaction.



Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

energized species

In an elementary process, a species having sufficient energy to become an activated complex, but which does not have the structure of the activated complex. If it is not inactivated by collisions it can become an activated complex and pass at once into products, after undergoing vibration.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 164

energy, E

In mechanics the sum of potential energy and kinetic energy. In thermodynamics the internal energy or thermodynamic energy increase, ΔU, is the sum of heat and work brought to the system. Only changes in energy are measurable. For photons

$$E = h\,\nu$$

where h is the Planck constant and ν the frequency of radiation. In relativistic physics

$$E = m\,c^2$$

where c is the speed of light and m the mass.

Source:
Green Book, 2nd ed., p. 12

energy dispersion

in emission spectrometry

The separation of characteristic photons according to their energy.

Source:
Orange Book, p. 180

energy dispersive X-ray fluorescence analysis

A method of X-ray fluorescence analysis where element specificity is obtained by measuring the energy spectrum of the induced X-radiation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

energy flux density

For mono-directional radiation, the energy traversing in a time interval over a small area perpendicular to the direction of the energy flow, divided by that time interval and by that area.
See also: intensity

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2519

energy gradient

First derivatives of the total energy with respect to nuclear coordinates, *i.e.*, negative values of forces on the nuclei. Evaluation of energy gradient plays a central role in searching potential energy surfaces for stationary points. A widespread technique is based on the minimization of the gradient norm (the square of energy gradient).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1938

energy hypersurface (synonymous with potential energy surface, PES)

The notion of hypersurface is used to stress the multidimensionality of PESs. In a molecular system consisting of N atomic nuclei, the number of the independent coordinates that fully determine the PES is equal to $3\,N-6$ (or $3\,N-5$ if the system is linear).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1938

energy migration

See: electronic energy migration

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2240

energy

of a radiation

Energy of the individual particles or photons of which a radiation consists.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518

energy of activation

See: activation energy

Source:
Green Book, 2nd ed., p. 55
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 164
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

energy of activation

of an electrode reaction

This is defined by the equation:

$$U^{\ddagger}=-R\,T\left(\frac{\partial(\ln I_0)}{\partial T^{-1}}\right)_{p,c_j,\dots}$$

where I_0 is the exchange current. At any overpotential η it is defined by the equation:

$$U^{\ddagger}(\eta) = -R\left(\frac{\partial(\ln(\,|\,I\,|\,))}{\partial T^{-1}}\right)_{p,\eta,c_j,\ldots}$$

where I is the current passing from the electrode into the electrolyte.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 516

energy profile

See: Gibbs energy diagram, potential-energy profile

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

energy resolution

in radiochemistry

A measurement, at given energy, of the smallest difference between the energies of two particles or photons capable of being distinguished by a radiation spectrometer.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2519

energy storage efficiency, η

The rate of the Gibbs energy storage in an endothermic photochemical reaction divided by the incident irradiance.
See also: efficiency

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2240

energy threshold

in radiochemistry

The limiting kinetic energy of a incident particle or energy of an incident photon below which a specified process cannot take place.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2519

energy transfer

in photochemistry

From a phenomenological point of view, the term is used to describe the process by which a molecular entity absorbs light and a phenomenon originates from the excited state of another molecular entity. In mechanistic photochemistry the term has been reserved for the photophysical process in which an excited state of one molecular entity (the donor) is deactivated to a lower-lying state by transferring energy to a second molecular entity (the acceptor) which is thereby raised to a higher energy state. The excitation may be electronic, vibrational, rotational or translational. The donor and acceptor may be two parts of the same molecular entity, in which case the process is called intramolecular energy transfer.
See also: Dexter excitation transfer, Förster excitation transfer, radiative energy transfer, spectral overlap

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2240

energy transfer plot

in photochemistry

A plot of the quenching rate constant of an excited molecular entity by a series of quenchers versus the excited state energy of the quenchers. Alternatively, a plot of the rate constant for the sensitization of a reaction versus the excited state energy of different sensitizers. This type of plot is used to estimate the energy of the excited molecular entity quenched (in the former case) or produced (in the latter case).
See also: Stern–Volmer kinetic relationships

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2240

energy yield of luminescence

The ratio of the energy emitted as luminescence to the energy absorbed by a species.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 243

enforced concerted mechanism

Variation of reaction parameters in a series of reactions proceeding in non-concerted steps may lead to a situation where the putative intermediate will possess a lifetime shorter than a bond vibration, so that the steps become concerted. The transition state structure will lie on the coordinate of the More O'Ferrall–Jencks diagram leading to that of the putative intermediate.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1112

enhanced phosphorescence analysis

in luminescence spectroscopy

A use of luminescence quenching effects to enhance sensitivity. The strong depopulation of the fluorescing singlet excited state by external heavy atom perturbers can lead to a large population of the phosphorescing triplet excited state.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 235

enhancement reaction

in analytical chemistry

A reaction which enables a favourable measurement to be made in which the constituent which is finally measured has not been magnified in any way (cf. amplification reaction).

Source:
PAC, 1982, *54*, 2553 *(Recommendations on use of the term amplification reactions)* on page 2556

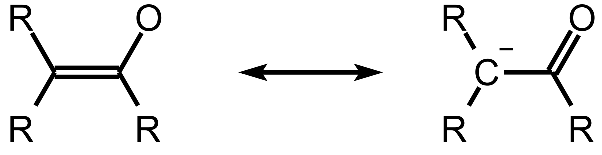
enhancer

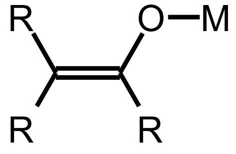
A fluorescent compound which accepts energy and thus enhances or promotes the emission from a sample containing a chemically or enzymatically generated excited molecular entity.
See also: dark photochemistry

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2240

enolates

Salts of enols (or of the tautomeric aldehydes or ketones), in which the anionic charge is delocalized over oxygen and carbon, or similar covalent metal derivatives in which the metal is bound to oxygen.





Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1334

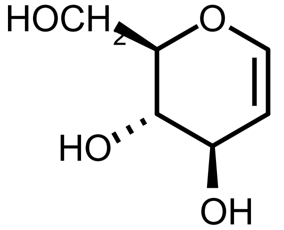
enols

Alkenols; the term refers specifically to vinylic alcohols, which have the structure $HOCR'=CR_2$. Enols are tautomeric with aldehydes (R' = H) or ketones (R' ≠ H).
See also: phenols

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1334

enoses

Monosaccharides having a carbon–carbon double bond anywhere in the backbone chain. Glycals (term not recommended) designates the enoses that are generated by formal elimination of the hemiacetal hydroxy group and an adjacent hydrogen atom. Thus glycals are cyclic enol ethers. Unsaturated hexoses, for example, are called hexenoses, e.g. the hex-1-enopyranose derived from D-glucopyranose):



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1334

enrichment factor, *S*

in liquid-liquid distribution

The factor by which the ratio of two substances in the feed must be multiplied to give their ratio after treatment.

$$\frac{Q_{\mathrm{A}}}{Q_{\mathrm{B}}} = S_{\mathrm{A,B}} \frac{Q'_{\mathrm{A}}}{Q'_{\mathrm{B}}}$$

where Q_{A} and Q'_{A} are the final and initial amounts of species **A** and Q_{B} and Q'_{A} are the final and initial amounts of species **B**. Hence $S_{\mathrm{A,B}} = \frac{E_{\mathrm{A}}}{E_{\mathrm{B}}}$ where E is the fraction extracted. In terms of D, n, r (where n is the number of stages and r the phase ratio),

$$S_{\mathrm{A,B}} = \frac{1 - (1 + r\,D_{\mathrm{A}})^{-n}}{1 - (1 + r\,D_{\mathrm{B}})^{-n}}$$

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2382
Orange Book, p. 90

ent

A prefix used to indicate the enantiomer for natural products and related molecules where the trivial name only refers to one enantiomer, e.g. *ent*-kaurene is the enantiomer of kaurene.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208

entanglement network

Polymer network with junction points or zones formed by physically entangled chains.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1814

entatic state

A state of an atom or group which, due to its binding in a protein, has its geometric or electronic condition adapted for function.
Note:
It is derived from entasis (Greek), meaning tension.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1272

entering group

An atom or group that forms a bond to what is considered to be the main part of the substrate during a reaction. For example: the attacking nucleophile in a bimolecular nucleophilic substitution reaction.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1113

enthalpimetric analysis

Synonym: analytical solution calorimetry

The generic designation for a family of analytical methods in which the enthalpy change of a chemical reaction is measured, directly or indirectly, in order to perform a quantitative determination of a reactant or catalyst. In general, at least one reactant is a liquid or solution. It is a subset of calorimetry in which the system is maintained at constant (usually atmospheric pressure), and the emphasis is on a quantitative determination in a reasonable length of time. Analytical solution calorimetry is a synonymous designation that may be used but is not preferred. Thermochemical analysis has been used but is not recommended because of potential confusion and overlap with the methods of thermal analysis. The adjective thermometric is also associated with the names of some of these methods, but is not recommended as a general designation.

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2489

enthalpimetry

See: enthalpimetric analysis

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2489

enthalpogram

A plot of temperature *versus* time or heat change *versus* time which is produced in direct-injection enthalpimetry. Use of the term thermogram is not recommended because it is too general and overlaps with other fields.

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2490

enthalpy, H

Internal energy of a system plus the product of pressure and volume. Its change in a system is equal to the heat brought to the system at constant pressure.

Source:
Green Book, 2nd ed., p. 48
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 972
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2187

enthalpy of activation, $\Delta^{\ddagger}H^{\circ}$

The standard enthalpy of activation $\Delta^{\ddagger}H^{\circ}$ is the enthalpy change that appears in the thermodynamic form of the rate equation obtained from conventional transition state theory. This equation is only correct for a first order reaction, for which the rate constant has the dimension reciprocal time. For a second order reaction, for which the rate constant has the dimension (reciprocal time) × (reciprocal concentration), the left hand side should be read as $k\,c^{\circ}$, where c° denotes the standard concentration (usually $1\ \mathrm{mol\ dm^{-3}}$).

$$k = \frac{k_{\mathrm{B}}T}{h}\,\mathrm{e}^{\frac{\Delta^{\ddagger}S^{\circ}}{R}}\,\mathrm{e}^{\frac{-\Delta^{\ddagger}H^{\circ}}{RT}}$$

The quantity $\Delta^{\ddagger}S^{\circ}$ is the standard entropy of activation, and care must be taken with standard states. In this equation k_{B} is the Boltzmann constant, T the absolute temperature, h the Planck constant, and R the gas constant. The enthalpy of activation is approximately equal to the activation energy; the conversion of one into the other depends on the molecularity. The enthalpy of activation is always the standard quantity, although the word standard and the superscript ° on the symbol are often omitted. The symbol is frequently (but incorrectly) written $\Delta H^{\ddagger}$, where the standard symbol is omitted and the ‡ is placed after the H.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 164
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1113
Green Book, 2nd ed., p. 56
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2294

enthalpy of immersion

Synonymous with enthalpy of wetting.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 605

enthalpy of wetting

Referred to unit of mass of the solid, the difference (at constant temperature) between the enthalpy of a solid completely immersed in a wetting liquid, and that of the solid and the liquid taken separately. It must be specified whether the solid in the initial state is in contact with vacuum or with the vapour of the liquid at a given partial pressure. Measurements of the enthalpy of wetting of a solid equilibrated with varying relative pressures of the vapour of a pure wetting liquid may be used to derive the differential enthalpy of adsorption of the vapour.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 605

entitic

Modifier used to denote divided by number of entities.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 972

entitic quantity

One which refers to a single entity (particle) of a system.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 441

entrainment

in atmospheric chemistry

The act of forming a mist or fog: droplets of a liquid carried off by the vapours of a boiling liquid or from a liquid through which bubbles of gas or vapour are passing rapidly.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2187

entrainment

in photochemistry

Term used in photostimulated radical nucleophilic substitution to designate the induction of the reaction of a less reactive (or non-reactive) nucleophile with a substrate by the addition of catalytic amounts of another nucleophile, more reactive at initiation. Often, the non-reactive nucleophile at initiation is, however, quite reactive at propagation.
Note:
Term also used in photobiology in connection with the setting of the circadian clock by biological photosensors such as phytochromes and cryptochromes in plants and cryptochromes in mammals and insects.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 335

entrance channel

The region of a potential-energy surface or hypersurface that corresponds to molecular configurations that are closer in geometry to those of the reactants than to those of the products.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 165

entropy, S

Quantity the change in which is equal to the heat brought to the system in a reversible process at constant temperature divided by that temperature. Entropy is zero for an ideally ordered crystal at 0 K. In statistical thermodynamics

$$S = k \ln W$$

where k is the Boltzmann constant and W the number of possible arrangements of the system.

Source:
Green Book, 2nd ed., p. 48
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2187
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 972

entropy of activation, $\Delta^{\ddagger}S^{\circ}$

The entropy change that appears in the thermodynamic form of the rate equation obtained from conventional transition-state theory.
See: enthalpy of activation

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 165
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1113

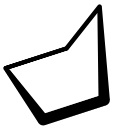
entropy unit

Non-SI unit of molar entropy, $\mathrm{e.u.} = 4.184\ \mathrm{J\ K^{-1}\ mol^{-1}}$.

Source:
Green Book, 2nd ed., p. 113

envelope conformation

The conformation (of symmetry group C_s) of a five-membered ring in which four atoms are coplanar, and one atom (the flap) projects out of the plane.



Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208

environmental (or ambient) monitoring

Continuous or repeated measurement of agents in the (working) environment to evaluate environmental exposure and possible damage by comparison with appropriate reference values based on knowledge of the probable relationship between ambient exposure and resultant health effects.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1022

environmental stress cracking

Cracking caused by the combined actions of (i) mechanical stress and (ii) chemical agents or radiation or both.

Source:
PAC, 1996, *68*, 2313 *(Definitions of terms relating to degradation, aging, and related chemical transformations of polymers (IUPAC Recommendations 1996))* on page 2318

enzyme activity

See: catalytic activity

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 972

enzyme induction

in general chemistry

The process whereby an (inducible) enzyme is synthesized in response to a specific molecule (cf. inducer).The inducer molecule (often a substrate that needs the catalytic activity of the inducible enzyme for its metabolism) combines with a repressor and thereby prevents the blocking of an operator by the repressor.

See also: enzyme induction (in medicinal chemistry)

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 152

enzyme induction

in medicinal chemistry

Process whereby an enzyme is synthesised in response to the presence of a specific substance or to other agents such as heat or a metal.
See also: enzyme induction (in general chemistry)

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1051

enzyme repression

The mode by which the synthesis of an enzyme is prevented by repressor molecules. In many cases, the end product of a synthesis chain (e.g. an amino acid) acts as a feed-back corepressor by combining with an intracellular aporepressor protein, so that this complex is able to block the function of an operator. As a result, the whole operon is prevented from being transcribed into mRNA, and the expression of all enzymes necessary for the synthesis of the end product amino acid is abolished.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 152

enzyme substrate electrode

A sensor in which an ion-selective electrode is covered with a coating containing an enzyme which causes the reaction of an organic or inorganic substance (substrate) to produce a species to which the electrode responds. Alternatively, the sensor could be covered with a layer of substrate which reacts with the enzyme, co-factor or inhibitor to be assayed.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2535

enzyme thermistor **[obsolete]**

See: flow injection enthalpimetry

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2491

enzymes

Macromolecules, mostly of protein nature, that function as (bio)catalysts by increasing the reaction rates. In general, an enzyme catalyses only one reaction type (reaction specificity) and operates on only one type of substrate (substrate specificity). Substrate molecules are attacked at the same site (regiospecificity) and only one or preferentially one of the enantiomers of chiral substrates or of racemic mixtures is attacked (stereospecificity).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 152
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2295
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

enzymic decomposition

Decomposition of organic materials (e.g. starch, sugars, proteins, etc.) can be achieved by enzymic decomposition, in which the enzyme converts a high molecular mass compound into lower molecular mass species. The process can be regarded as an example of enzymic degradation.

Source:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1469

epi-phase

The less dense phase in a distribution system. The term is often used when two non-aqueous phases are present or when the solvent is an aqueous solution.
See also: hypo-phase

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2380

epicadmium neutrons

Neutrons of kinetic energy greater than the effective cadmium cut-off energy.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

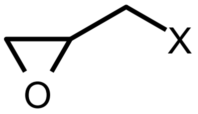
epigenetic

Descriptive term for processes that change the phenotype without altering the genotype.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 153

epihalohydrins

Compounds having the (halomethyl)oxirane skeleton:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1334

epimerization

Interconversion of epimers.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1114

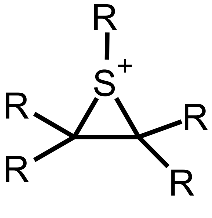
epimers

Diastereoisomers that have the opposite configuration at only one of two or more tetrahedral stereogenic centres present in the respective molecular entities.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1113

episulfonium ions

Ions derived from thiiranes, in which a trivalent sulfur atom bears a positive charge:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1334

epithermal neutrons

Neutrons of kinetic energy greater than that of thermal agitation. The term is often restricted to energies just above thermal.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

epitope

Any part of a molecule that acts as an antigenic determinant. A macromolecule can contain many different epitopes each capable of stimulating production of a different specific antibody.

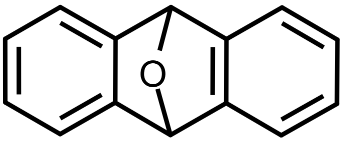
Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 153

epoxy compounds

Also contains definition of: epoxides

Compounds in which an oxygen atom is directly attached to two adjacent or non-adjacent carbon atoms of a carbon chain or ring system; thus cyclic ethers. The term epoxides represents a subclass of epoxy compounds containing a saturated three-membered cyclic ether; thus oxirane derivatives, e.g. 1,2-epoxypropane, or 2-methyloxirane (an epoxide); 9,10-epoxy-9,10-dihydroanthracene (an epoxy compound).

1,2-epoxypropane



9,10-epoxy-9,10-dihydroanthracene

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1334

equalization of electronegativity, principle of

The postulate that in a molecule all the constituent atoms should have same electronegativity value, which would be the geometric mean of the electronegativities of isolated atoms.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1938

equatorial

1. For the use of this term in the context of cyclohexane see axial, equatorial.
2. For the use of this term in the context of a bipyramidal structure see apical, basal, equatorial.

   Source:
   PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208

equilibration

The operation by which a system of two or more phases is brought to a condition where further changes with time do not occur. This term is not synonymous with pre-equilibrium and should not be used in that sense.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2377

equilibrium constant

Quantity characterizing the equilibrium of a chemical reaction and defined by an expression of the type $K_x = \prod_{\mathrm{B}} {x_{\mathrm{B}}}^{\nu_{\mathrm{B}}}$, where ν_{B} is the stoichiometric number of a reactant (negative) or product (positive) for the reaction and x stands for a quantity which can be the equilibrium value either of pressure, fugacity, amount concentration, amount fraction, molality, relative activity or reciprocal absolute activity defining the pressure based, fugacity based, concentration based, amount fraction based, molality based, relative activity based or standard equilibrium constant (then denoted K°), respectively.

Source:
Green Book, 2nd ed., p. 50

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2187

PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 972

equilibrium dialysate

The colloid-free solution obtained at equilibrium in dialysis. Its composition approaches that of the dispersion medium (more precisely, the limit to which the composition of the dispersion medium tends at large distances from the particles). In the dialysis equilibrium an osmotic pressure difference exists between sol and equilibrium dialysate.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

equilibrium distance

in a molecule

Internuclear distance at the minimum of the electronic (or potential) energy surface.

Source:
Green Book, 2nd ed., p. 24

equilibrium film

A liquid film of thickness, or thicknesses, at which it is stable or metastable with respect to small thickness changes. Unless the area of the film is small, its composition may not be the same over its area and the (metastable) equilibrium thickness may be characteristic of the local condition only.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 614

equilibrium geometry

Molecular geometry that corresponds to the true minimum on the respective potential energy surface. While information relating to the equilibrium geometry is provided by calculations within the adiabatic approximation (minimization of the total energy with respect to any independent geometrical parameter), various experiments yield some effective geometries for the molecule which are averaged over molecular vibrations.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1938

equilibrium reaction

When the reactants in a chemical reaction are initially in a Boltzmann distribution the reaction is referred to as an equilibrium reaction.
See also: non-equilibrium reaction

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 165

equilibrium sedimentation

A method by which the distribution of the concentration of the solute or dispersed component in a dilute solution or dispersion along the centrifuge cell is measured at sedimentation equilibrium and the results are interpreted in terms of molar masses or their distribution, or both.

Source:
Purple Book, p. 62

equivalence postulate

in polymer chemistry

The working hypothesis that the chain monomeric units are geometrically equivalent.

Source:
Purple Book, p. 78

equivalent chain

in polymers

A hypothetical freely jointed chain with the same mean-square end-to-end distance and contour length as an actual polymer chain in a theta state.

Source:
Purple Book, p. 50

equivalent diameter

The diameter of a spherical particle which will give identical geometric, optical, electrical or aerodynamic behaviour to that of the particle (non-spherical) being examined; sometimes referred to as the Stokes diameter for particles in non-turbulent flows.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2184

equivalent entity

Entity corresponding to the transfer of a H^+ ion in a neutralization reaction, of an electron in a redox reaction, or to a magnitude of charge number equal to 1 in ions. Examples: $\frac{1}{2}$ H_2SO_4, $\frac{1}{5}$ $KMnO_4$, $\frac{1}{3}$ Fe^{3+}.

Source:
Physical Chemistry Division, unpublished

erg

cgs unit of energy, $\mathrm{erg} = 10^{-7}\ \mathrm{J}$.

Source:
Green Book, 2nd ed., p. 112
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 973

error

of measurement

Result of a measurement minus the true value of the measurand. Since a true value cannot be determined, in practice the conventional true value is used.
See also: measurement result

Source:
VIM
Orange Book, p. 6
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 601

erythro*, *threo

Descriptors of the diastereoisomers of an acyclic structure or partial structure having two stereogenic centres. This notation is derived from carbohydrate nomenclature. The extension of this system has given rise to conflicting interpretations of these prefixes. It is recommended that for such cases the l, u or R^*, S^* system should be used.

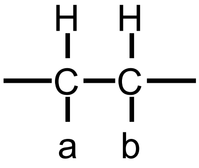
Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208

***erythro* structures**

Also contains definition of: *threo* structures *in a polymer*

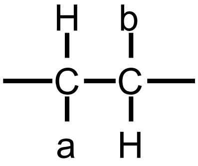
in a polymer

The relative configuration at two contiguous carbon atoms in the main chain bearing, respectively, substituents a and b (a ≠ b), is designated by the prefix *erythro* or *threo*, as appropriate, by analogy with the terminology for carbohydrate systems in which the substituents are OH. Examples:



$$-\overset{\displaystyle H}{\underset{\displaystyle a}{C}}-\overset{\displaystyle H}{\underset{\displaystyle b}{C}}-$$

erythro



$$-\overset{\displaystyle H}{\underset{\displaystyle a}{C}}-\overset{\displaystyle b}{\underset{\displaystyle H}{C}}-$$

threo

Similar systems in which a higher level of substitution exists may be treated analogously if the *erythro* or *threo* designation is employed to denote the relative placements of those two substituents, one for each backbone carbon atom, which rank highest according to the Sequence Rule.

Source:
Purple Book, p. 36

escape depth (for surface analysis techniques)

The distance into the sample measured from the physical surface from which all but a fraction $\frac{1}{e}$ of the particles or radiation detected have originated.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

Esin and Markov coefficient

The left-hand side of one of the various cross-differential relationships that can be obtained from the Gibbs adsorption equation when only one chemical potential (μ) is considered as variable, viz.

$$\left(\frac{\partial E}{\partial \mu}\right)_{T,p,\sigma} = -\left(\frac{\partial \Gamma}{\partial \sigma}\right)_{T,p,\mu}$$

where E is the potential difference, T is the temperature, p is the pressure, Γ is the surface excess and σ is the charge density.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 446

esters

Compounds formally derived from an oxoacid $R_kE(=O)_l(OH)_m$, ($l \neq 0$) and an alcohol, phenol, heteroarenol, or enol by linking with formal loss of water from an acidic hydroxy group of the former and a hydroxy group of the latter. By extension acyl derivatives of alcohols, etc. Acyl derivatives of chalcogen analogues of alcohols (thiols, selenols, tellurols) etc. are included. E.g. R'C(=O)(OR) , R'C(=S)(OR) , R'C(=O)(SR) , $R'S(=O)_2(OR)$, $(HO)_2P(=O)(OR)$, $(R'S)_2C(=O)$, ROCN (but not R–NCO) ($R \neq H$).
Note:
O-Alkyl derivatives of other acidic compounds [see amides (1)] may be named as esters but do not belong to the class esters proper. E.g. $(Ph)_2POCH_3$ methyl diphenylphosphinite.
See also: acylals, ortho esters, depsides, depsipeptides, glycerides, lactides, lactones, macrolides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1334

E_T-value

See: Dimroth–Reichardt E_T parameter, Z-value

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1108

ethers

Compounds ROR ($R \neq H$). (Compounds R_3SiOR, silicon analogues of ethers, are trialkylsilyloxy compounds). E.g. $CH_3CH_2OCH_2CH_3$,
See also: acetals, epoxy compounds, ortho esters

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1334

euatmotic reaction

An isothermal, reversible reaction between two (or more) solid phases during the heating of a system as a result of which a single vapour phase is produced.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 582

eupeptide bond

See: peptide

Source:
White Book, p. 48

eutectic reaction

An isothermal, reversible reaction between two (or more) solid phases during the heating of a system, as a result of which a single liquid phase is produced.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 582

evaluation function

The inverse of the calibration function.

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1704

evaporation

The physical process by which a liquid substance is converted to a gas or vapour. This may occur at or below the normal boiling point of the liquid (the temperature at which a liquid boils at 1 atmosphere pressure) and the process is endothermic.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

even-electron ion

An ion containing no unpaired electrons, for example CH_3^+ in its ground state.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

evolved gas analysis (EGA)

A technique in which the nature and/or amount of volatile product(s) released by a substance subjected to a controlled temperature program is (are) determined. The method of analysis should always be clearly stated.

Source:
Orange Book, p. 42

evolved gas detection (EGD)

A technique in which the evolution of gas from a substance is detected as a function of temperature while the substance is subjected to a controlled temperature program.

Source:
Orange Book, p. 41

Ewens–Bassett number [obsolete]

Usage no longer recommended.
See: oxidation number, charge number

Source:
Red Book, p. 66

exa

SI prefix for 10^{18} (symbol: E).

Source:
Green Book, 2nd ed., p. 74

excess acidity

See: Bunnett–Olsen equations, Cox–Yates equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1114

excess Rayleigh ratio

The difference between the Rayleigh ratio for a dilute solution and for pure solvent. If the scattering intensity is not reduced to the Rayleigh ratio, the difference between the scattering intensities for a dilute solution and that for pure solvent is named 'excess scattering'.

Source:
Purple Book, p. 66

excess volume (at a solid/liquid interface)

Also contains definition of: excess mass (at a solid/liquid interface)

For a pure liquid, despite its low compressibility, the variation of density near a solid surface can be detected and measured. The total volume V of a system consisting of solid and pure liquid is different from (usually less than) that calculated assuming a constant liquid density. If the densities of bulk solid (ρ^{sol}) and liquid (ρ^{l}) are known then an excess volume (usually negative) can be defined as:

$$V^{\sigma} = V - V^{\mathrm{sol}} - V^{\circ} = V - \frac{m^{\mathrm{sol}}}{\rho^{\mathrm{sol}}} - \frac{m^{\mathrm{l}}}{\rho^{\mathrm{l}}}$$

where m^{sol} is the mass of solid, V^{sol} its volume calculated from the bulk density, V° is the initial volume of liquid and m^{l} is the mass of liquid. The excess mass is given by:

$$m^{\sigma} = m^{\mathrm{l}} - (V - V^{\mathrm{sol}})\, \rho^{\mathrm{l}}$$

Source:
PAC, 1986, *58*, 967 *(Reporting data on adsorption from solution at the solid/solution interface (Recommendations 1986))* on page 972

exchange current

of an electrode reaction

The common value I_0 of the anodic and cathodic partial currents when the reaction is at equilibrium

$$I = I_{\mathrm{a}} = -I_{\mathrm{c}}$$

For an electrode at equilibrium at which only one reaction is significant $I = 0$. When more than one reaction is significant at a given electrode, subscripts to I_0 may be used to distinguish exchange currents. I is not usually zero when only one of these reactions is at equilibrium.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 513

exchange extraction

An extraction operation or process in which a metal from one phase is exchanged with the equivalent amount of a second metal from the other phase.
Notes:

1. This term may be used in connection with any step (e.g. loading, scrubbing or stripping in a process).
2. This applies also to organic or molecular species.

See also: crowding

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2387

exchange labelling

Labelling of a substance by isotope exchange.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

exchange repulsion

Also contains definition of: exchange integral

The correction to the Coulomb repulsion between two electrons in orbitals Ψ_i and Ψ_j for the case when the electrons possess parallel spins. It is to be subtracted from the Coulomb repulsion to give the total energy of the electron–electron interaction. In the Hartree–Fock theory the magnitude of the exchange repulsion is given by the exchange integral

$$K_{ij} = \int\int \Psi_i^*(\mathbf{r}_1)\, \Psi_j^*(\mathbf{r}_1) \left(\frac{e^2}{r_{12}}\right) \Psi_i(\mathbf{r}_2)\, \Psi_j(\mathbf{r}_2) \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 = \; < ij \mid ji >$$

For the case of electrons with opposite spins K_{ij} vanishes.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1938

exchange-inversion transition

A transition between antiferromagnetic and ferromagnetic coupling between two subarrays of magnetic atoms. Example: Ordered FeRh changes from antiferromagnetic to ferromagnetic coupling with the simple cubic Fe array in a first-order transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 582

excimer

An electronically excited dimer, 'non-bonding' in the ground state. For example, a complex formed by the interaction of an excited molecular entity with a ground state partner of the same structure.
See also: exciplex

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2240
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1114

excimer lamp

Non-coherent source of *ultraviolet* radiation capable of producing quasi-monochromatic radiation from the near UV ($\lambda = 354\ \mathrm{nm}$) to the vacuum UV ($\lambda = 126\ \mathrm{nm}$). The operation of the excimer lamps relies on the radiative decomposition of *excimers* or *exciplexes* created by various types of discharges.
Notes:

1. Using noble gas, halogen, or noble gas / halogen mixtures with fill pressure ~ 30 kPa, the radiative decomposition of the excimer or the exciplex produces nearly monochromatic radiation. Some of the commercially available wavelengths for the particular excimers or exciplexes are 126 nm with Ar_2, 146 nm with Kr_2, 172 nm with Xe_2, 222 nm with KrCl, and 308 nm with XeCl, obtained with efficiencies of 5 - 15 %. Pulsed Xe-excimer (Xe_2) lamps may have up to 40 % efficiency. Good efficiencies are also obtained with XeBr at 291 nm and with XeI at 253 nm. Other wavelengths produced with much less efficiency are 207 nm (KrBr), 253 nm (XeI), 259 nm (Cl_2), and 341 nm (I_2) (see Table 1).

   Table 1: Peak wavelengths (nm) obtained in dielectric-barrier discharges with mixtures of noble gas (Ng) and halogen (X_2). Wavelengths of commercially available lamps are shown in boldface type. The molecular species indicated are excimers or exciplexes.

	X_2	Ne	Ar	Kr	Xe
Ng_2			**126**	**146**	**172**
F	157	108	193	249	354
Cl	259		175	**222**	**308**
Br	291		165	207	283
I	341			190	253

2. Phosphors are used to transform the UV radiation into visible radiation. This is the basis of mercury-free fluorescent lamps and of flat plasma-display panels with a large screen.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 335

excimer laser

A source of pulsed coherent radiation obtained from an exciplex. The proper name is exciplex laser. Typical lasing species are noble gas halides (XeCl, KrF, etc.) emitting in the UV domain.
See: gas lasers

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2241
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1920

excimer-luminescence

in luminescence quenching

An effect accompanying concentration quenching in some cases, namely the formation of a new bimolecular species which is capable of emission (excimer- and exciplex-luminescence).

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 235

excipient

in toxicology

Any more or less inert substance added to a drug to give suitable consistency or form to the drug.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2046

exciplex

An electronically excited complex of definite stoichiometry, 'non-bonding' in the ground state. For example, a complex formed by the interaction of an excited molecular entity with a ground state counterpart of a different structure.
See also: excimer

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1114

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2241

exciplex-luminescence

in luminescence quenching

See: excimer-luminescence *in luminescence quenching*

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 235

excitation

Process causing the transition of a system from one state to another of higher energy.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

excitation energy

The minimum energy required to bring a system to a specified higher energy level.

Source:
Orange Book, p. 223

excitation energy

Synonym: initial energy *in in situ microanalysis*

in in situ microanalysis

Sometimes called acceleration energy or initial energy. Kinetic energy of bombarding particles at the surface of the solid.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2027

excitation level

in X-ray spectroscopy

X-ray levels have various degrees of ionization -- single, double or higher -- and may in some cases also be electrically neutral. An excitation level (exciton) is an electrically neutral X-ray level with an expelled electron bound in the field of a core electron vacancy.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 738

excitation spectrum

A plot of the spectral radiant exitance or of the spectral photon exitance against the frequency (or wavenumber, or wavelength) of excitation. When corrected for wavelength dependent variations in the excitation radiant power this is called a corrected excitation spectrum.
See also: emission spectrum

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2241

See also:
Orange Book, p. 197

excitation transfer

Synonymous with energy transfer.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2241

excitation-emission spectrum

The three-dimensional spectrum generated by scanning the emission spectrum at incremental steps of excitation wavelength (x axis = emission wavelength, y axis = excitation wavelength, z axis =

emission flux) is called a (fluorescence, phosphorescence) excitation-emission spectrum (or EES). The spectra are particularly useful for investigating samples containing more than one emitting species. Corrected EES are obtained if (a) the emission is corrected for instrumental response with wavelength, and (b) the exciting radiation flux in photons s^{-1} is held constant for all excitation wavelengths.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 242

excited state

State of a system with energy higher than that of the ground state. This term is most commonly used to characterize a molecule in one of its electronically excited states, but can also refer to vibrational and/or rotational excitation in the electronic ground state.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1114
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2241

exciton

In some applications it is useful to consider electronic excitation as if a quasi-particle, capable of migrating, were involved. This is termed an exciton. In organic materials two models are used: the band or wave model (low temperature, high crystalline order) and the hopping model (higher temperature, low crystalline order or amorphous state). Energy transfer in the hopping limit is identical with energy migration.
See: electronic energy migration

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2241

excluded volume of a macromolecule

in polymers

The volume from which a macromolecule in a dilute solution of a macromolecule effectively excludes all other macromolecules. The excluded volume of a macromolecule depends on the Gibbs and Helmholtz energies of mixing of solvent and polymer, i.e. on the thermodynamic quality of the solvent, and is not a measure of the geometrical volume of that macromolecule.

Source:
Purple Book, p. 58

excluded volume of a segment

in polymers

The volume from which a segment of a macromolecule in solution effectively excludes all other segments, i.e. those belonging to the same macromolecule as well as those belonging to other macromolecules. The excluded volume of a segment depends on the Gibbs and Helmholtz energies of mixing of solvent and polymer, i.e. on the thermodynamic quality of the solvent, and is not a measure of the geometrical volume of that segment.

Source:
Purple Book, p. 58

exclusion chromatography

Chromatography in which separation is based mainly on exclusion effects, such as differences in molecular size and/or shape or in charge. The term size-exclusion chromatography may also be used when separation is based on molecular size. The terms gel filtration and gel-permeation chromatography (GPC) were used earlier to describe this process when the stationary phase is a swollen gel. The term ion-exclusion chromatography is specifically used for the separation of ions in an aqueous phase.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 826

exergonic (exoergic) reaction

This expression is often applied to a reaction for which the overall standard Gibbs energy change ΔG° is negative. Some workers use this term with reference to a negative value of ΔH° at the absolute zero of temperature.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 165

exfoliated graphite

The product of very rapid heating (or flash heating) of graphite intercalation compounds, such as graphite hydrogensulfate of relatively large particle diameter (flakes). The vaporizing intercalated substances force the graphite layers apart. The exfoliated graphite assumes an accordion-like shape with an apparent volume often hundreds of times that of the original graphite flakes.
Note:
Exfoliated graphite is usually prepared from well-crystallized natural flake graphite. It is used for the production of graphite foils. Exfoliated graphite is different from the deflagration product of graphite oxide (graphitic acid).

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 488

exfoliation

Process by which the layers of a multi-layered structure separate.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1822

exit channel

This expression refers to the region of a potential-energy surface or hypersurface that corresponds to molecular configurations that are closer to those of the products than to those of the reactants.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 165

exitance

See: radiant exitance

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2241

exoenzymes

Enzymes that cleave monomers (sometimes also di- or oligomers) from one end of a polymer chain. Exonucleases are able to cleave nucleotides, one by one, from either the 5- or the 3- (or both) ends of nucleic acids.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 153

exon

A section of DNA which carries the coding sequence for a protein or part of it. Exons are separated by intervening, non-coding sequences (cf. intron). In eukaryotes most genes consist of a number of exons.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 153

exothermic reaction

A reaction for which the overall standard enthalpy change ΔH° is negative.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 165

expansion factor

in polymers

The ratio of a dimensional characteristic of a macromolecule in a given solvent at a given temperature to the same dimensional characteristic in the θ state at the same temperature. The most frequently used expansion factors are: expansion factor of the mean-square end-to-end distance, $\alpha_r = \sqrt{\frac{< r^2 >}{< r^2 >_0}}$; expansion factor of the radius of gyration $\alpha_s = \sqrt{\frac{< s^2 >}{< s^2 >_0}}$; viscosity expansion factor $\alpha_\eta = \left(\frac{[\eta]}{[\eta]_\theta}\right)^{\frac{1}{3}}$ where $[\eta]$ and $[\eta]_\theta$ are the intrinsic viscosity in a given solvent and in the θ state at the same temperature, respectively. Expansion factors defined by different dimensional characteristics are not exactly equal, nor need they have a constant ratio as a function of relative molecular mass.

Source:
Purple Book, p. 59

experimental perturbational calculation

To assess the uncertainty of derived final results from a least-squares procedure one can investigate the sensitivity of output data for errors in the input data by means of this calculation. One performs the calculations many times with perturbed input data and studies the relation between the changes (perturbations) in the input data and the changes in the output data. The perturbations are preferably generated using random numbers with a distribution function chosen to mimic the distribution of uncertainties in the primary results.
See also: least-squares technique

Source:
PAC, 1981, *53*, 1805 *(Assignment and presentation of uncertainties of the numerical results of thermodynamic measurements (Provisional))* on page 1823

explosivity limits (explosion limits)

The concentration limits, usually of a substance in air, between which combustion will be self-sustaining.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

exponential decay

Variation of a quantity (generally the activity of a quantity of a radionuclide) according to the law $A = A_0\,\mathrm{e}^{-\lambda t}$ where A and A_0 are the values of the quantity being considered at time t and zero respectively, and λ is an appropriate constant.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

exposure

in medicinal chemistry

1. Concentration, amount or intensity of a particular physical or chemical agent or environmental agent that reaches the target population, organism, organ, tissue, or cell, usually expressed in numerical terms of concentration, duration, and frequency (for chemical agents and micro-organisms) or intensity (for physical agents).
2. Process by which a substance becomes available for absorption by the target population, organism, organ, tissue or cell, by any route.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1051
N.B. This differs from the definition of exposure in radiation chemistry.

exposure

in nuclear chemistry

For X- or gamma-radiation in air: the sum of the electrical charges of all the ions of one sign produced when all electrons liberated by photons in a suitably small element of volume of air completely stopped, divided by the mass of the air in the volume element.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541
This definition replaces an earlier definition of exposure.

exposure

in photochemistry

Term generally applied to the time-integrated radiation incident from all upward directions on a small sphere divided by the cross-sectional area of that sphere.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 338

expression

in biotechnology

1. The cellular production of the protein encoded by a particular gene. The process includes transcription of DNA, processing of the resulting mRNA product and its translation into an active protein.
2. A recombinant gene inserted into a host cell by means of a vector is said to be expressed if the synthesis of the encoded protein can be demonstrated.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 153

extended Hammett equation

This term applies in a general way to any multiparametric extension of the Hammett equation. It is sometimes used specifically for a form of dual substituent-parameter equation in which the actual value of the correlated property P under the influence of the substituent X is used, rather than the value relative to that for X = H. An intercept term h corresponding to the value of P for X = H is introduced, e.g.

$$P = \alpha\,\sigma_I + \beta\,\sigma_R + h$$

The equation may be applied to systems for which the inclusion of further terms to represent other effects, e.g. steric, is appropriate.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1114

extended Hückel MO method (EHMO)

A semi-empirical all-valence electron quantum mechanical method which uses the same approximations, apart from π-approximation and neglect of overlap integrals, as those of the Hückel molecular orbital theory. The method reproduces relatively well the shapes and the order of energy levels of molecular orbitals. The account for overlap makes it possible to describe the net destabilization caused by interaction of two doubly occupied orbitals, which effect is not reproduced by HMO theory.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1939

extended X-ray absorption fine structure (EXAFS)

Structure in X-ray absorption spectra remote from the edge and extending to higher energies, due mainly to the scattering of the expelled electron by neighbouring atoms. Structure closer to the absorption edge is sometimes called near-edge X-ray absorption fine structure (NEXAFS).

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 738

extended-chain crystal

in polymers

A polymer crystal in which the chains are in an essentially fully extended conformation.

Source:
Purple Book, p. 84

extender

Substance, especially a diluent or modifier, added to a polymer to increase its volume without substantially altering the desirable properties of the polymer.
Note:
An extender may be a liquid or a solid.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1995

extensive quantity

Physical quantity whose magnitude is additive for subsystems.

Source:
Green Book, 2nd ed., p. 7
PAC, 1986, *58*, 1405 *(Recommendations for the presentation of thermodynamic and related data in biology (Recommendations 1985))* on page 1407

extent of an interface (surface)

Also contains definitions of: geometric surface (interface) area, stepped surface

A quantity measured by its area, A (or S). For solids, a real (true, actual) and a geometric surface (interface) area, A_r and A_g, respectively, may be defined if asperities are present whose height is orders of magnitude greater than the atomic or molecular size. The geometric surface is the projection of the real surface on a plane parallel to the macroscopic, visible phase boundary. If asperities are of the order of the atomic size, the surface of the solid may be described as stepped. (High index faces of crystals are stepped surfaces but may be ideally smooth in the sense of the roughness factor.)

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

extent of reaction, ξ

Extensive quantity describing the progress of a chemical reaction equal to the number of chemical transformations, as indicated by the reaction equation on a molecular scale, divided by the Avogadro constant (it is essentially the amount of chemical transformations). The change in the extent of reaction is given by $\mathrm{d}\xi = \frac{\mathrm{d}n_\mathrm{B}}{\nu_\mathrm{B}}$, where ν_B is the stoichiometric number of any reaction entity **B** (reactant or product) and $\mathrm{d}n_\mathrm{B}$ is the corresponding amount.

Source:
Green Book, 2nd ed., p. 43
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 165
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 973
PAC, 1992, *64*, 1569 *(Quantities and units for metabolic processes as a function of time (IUPAC Recommendations 1992))* on page 1572
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2295

external compensation **[obsolete]**

The absence of optical activity in a racemate. (Usage strongly discouraged).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208

external heavy atom effect

See: heavy atom effect

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2241

external ion return

See: ion-pair return

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1127

external return

See: ion-pair return

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1114

external standard

in chromatography

A compound present in a standard sample of known concentration and volume which is analysed separately from the unknown sample under identical conditions. It is used to facilitate the qualitative indentification and/or quantitative determination of the sample components. The volume of the external standard (standard sample) need not to be known if it is identical to that of the unknown sample.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 837

external surface

When a porous solid consists of discrete particles it is inconvenient to describe the outer boundary of the particles as the external surface.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 585
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

exterplex **[obsolete]**

Termolecular analogue of an exciplex. Use of this term is discouraged.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2242

extinction **[obsolete]**

This term, sometimes used as equivalent to absorbance, is no longer recommended.
See: attenuance

Source:
Green Book, 2nd ed., p. 32
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2242
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 973

extinction coefficient [obsolete]

See: attenuation coefficient

Source:
Green Book, 2nd ed., p. 32
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2242
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 973

extra-column volume

in chromatography

The volume between the effective injection point and the effective detection point, excluding the part of the column containing the stationary phase. It is composed of the volumes of the injector, connecting lines and detector.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 832

extract (noun)

The separated phase (often but not necessarily organic) that contains the material extracted from the other phase. Where appropriate the term 'loaded solvent' may be used, but is not recommended.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2380
Orange Book, p. 91

extract (verb)

To transfer a solute from a liquid phase to another immiscible or partially miscible liquid phase in contact with it. The term is also applied to the dissolution of material from a solid phase with a liquid in which it is not wholly soluble (i.e. leaching).
See also: solvent extraction

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2377
Orange Book, p. 95

extractability

in solvent extraction

A property which qualitatively indicates the degree to which a substance is extracted. The term is imprecise and generally used in a qualitative sense. It is not a synonym for fraction extracted.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2382

extractant

Synonym: extracting agent

The active component(s) primarily responsible for transfer of a solute from one phase to the other.
Notes:

1. The term extracting agent is a synonym but solvent and ligand should not be used in this context.
2. Certain extractants that consist of liquids immiscible with water (e.g. tributyl phosphate or certain ketones) might comprise the only component of the initial organic phase but extractant(s) can also be dissolved in diluent.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2380
Orange Book, p. 91

extraction

Distribution and partition are often used as synonyms for the general phenomenon of extraction where appropriate.
See: liquid-liquid extraction

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2377

extraction coefficient [obsolete]

This term is not recommended as a synonym for distribution ratio.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2382
Orange Book, p. 89

extraction (equilibrium) constant

The extraction constant at zero ionic strength, K_{ex}^{0}, is the equilibrium constant of the distribution reaction expressed in terms of the reacting species. Thus, for the gross reaction:

$$\mathrm{M}_{\mathrm{aq}}^{n+} + n\mathrm{HL}_{\mathrm{org}} \rightleftarrows \mathrm{ML}_{n,\,\mathrm{org}} + n\mathrm{H}_{\mathrm{aq}}^{+}$$

in which the reagent HL initially dissolved in an organic phase reacts with a metal ion M^{n} in aqueous solution to form a product ML_n which is more soluble in the organic phase than in water,

$$K_{\mathrm{ex}}^{0} = \frac{a_{\mathrm{ML}\,n,\,\mathrm{org}}\; a_{\mathrm{H}^{+},\,\mathrm{aq}}^{n}}{a_{M^{n+},\,\mathrm{aq}}\; a_{\mathrm{HL}\,,\,\mathrm{org}}^{n}}$$

Notes:

1. When concentrations are used instead of activities or mixed terms are employed as when H^{+} and/or M^{n} are measured with an electrode, the appropriate name is extraction constant, symbol K_{ex}, accompanied by a careful definition. K_{ex}^{0} may be termed the thermodynamic extraction constant.
2. The extraction constant is related to other terms relevant to such systems by:

   $$K_{\mathrm{ex}} = \frac{D_{\mathrm{ML}\,n}\, \beta_n\, K_a^{n}}{D_{\mathrm{HL}}{}^{n}}$$

   where β_n is the overall formation constant of ML_n and K_a is the dissociation constant of HL. Where the reagent HL is more soluble in water than the other immiscible phase it may be more convenient to define a special equilibrium constant in terms of HL_{aq}:

   $$K_{\mathrm{ex}} = D_{\mathrm{ML}\,n}\, \beta_n\, K_a{}^{n}$$
3. In distribution equilibria involving non-aqueous systems, e.g. liquid $\mathrm{SO_2}$, molten salts and metals, the mass action equilibrium constant for the relevant extraction process can be identified with K_{ex} which should be explicitly defined in this context.
4. In actual practice, it may be necessary to include other terms to take into account other complexes formed by auxiliary reagents and the solvation and/or polymerization of the various species. In such cases, K_{ex} must be defined with reference to the relevant explicit chemical equation. An example is complex formation between the metal ion and an uncharged crown ether or cryptand molecule followed by ion-pair extraction:

   $$\mathrm{M}_{\mathrm{aq}}^{n+} + \mathrm{L}_{\mathrm{org}} + n\mathrm{A}_{\mathrm{aq}}^{-} \rightleftarrows (\mathrm{ML}^{n+}.\mathrm{A}_{n}^{n-})_{\mathrm{org}}$$

   $$K_{\mathrm{ex}} = \frac{[\mathrm{ML}^{n+}\mathrm{A}_{n}^{n-}]_{\mathrm{org}}}{[\mathrm{M}^{n+}]_{\mathrm{aq}}\, [\,\mathrm{L}\,]_{\mathrm{org}}\, [\mathrm{A}^{-}]_{\mathrm{aq}}{}^{n}}$$
5. Use of Ringbom's 'conditional extraction constant',

   $$K_{\mathrm{ex}}^{\mathrm{eff}} = \frac{a_{\mathrm{H}^{+}}^{n}{}^{n}\, [\mathrm{ML}_{n}']_{\mathrm{org}}}{[\mathrm{M}']_{\mathrm{aq}}\, [\mathrm{HL}']_{\mathrm{org}}{}^{n}}$$

in conjunction with alpha coefficients is useful.
6. The phases can also be specified by the formula of the solvent or by other symbols (preferably Roman numerals) or by overlining formulae referring to one phase, usually the less polar one. The subscript aq (or w) is often omitted; aq is preferable to w as the latter is appropriate only in English and German.
7. The qualification 'equilibrium' is often omitted.
8. The terms partition constant and distribution constant must not be used in this sense.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2383
Orange Book, p. 89

extraction factor, D_m

Synonym: mass distribution ratio

The ratio of the total mass of a solute in the extract to that in the other phase.
Notes:
1. It is the product of the (concentration) distribution ratio and the appropriate phase ratio.
2. It is synonymous with the concentration factor or mass distribution ratio, this latter term being particularly apt.
3. The term concentration factor is often employed for the overall extraction factor in a process or process step.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2384

extraction fractionation

of polymers

A process in which a polymeric material, consisting of macromolecules differing in some characteristic affecting their solubility, is separated from a polymer-rich phase into fractions by successively increasing the solution power of the solvent, resulting in the repeated formation of a two-phase system in which the more soluble components concentrate in the polymer-poor phase.

Source:
Purple Book, p. 68

extraction

in process liquid-liquid distribution

In connection with processes, this term often refers to the initial transfer step whereby the main solute, often together with impurities, is transferred from feed to solvent.
Notes:
1. Partition and distribution are not synonymous in this specific instance.
2. The term extraction may be used in a more general sense.

See also: loading

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2387

extraction isotherm

See: distribution isotherm

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2387

extrapolated range

in radiochemistry

The distance from a radiation source, calculated by extrapolation to zero of the flux density, of the tangent to the flux density versus distance curve, taken at the point where the flux density has decreased to one half of its initial value.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

extremophiles

Organisms which require extreme physico-chemical conditions for their optimum growth and proliferation. Extremophilic microorganisms are e.g. thermophiles or psychrophiles, halophiles, alkalophiles or acidophiles, osmophiles and barophiles, based on their growth at extremes of temperature, salt concentration, pH, osmolarity or pressure, respectively.

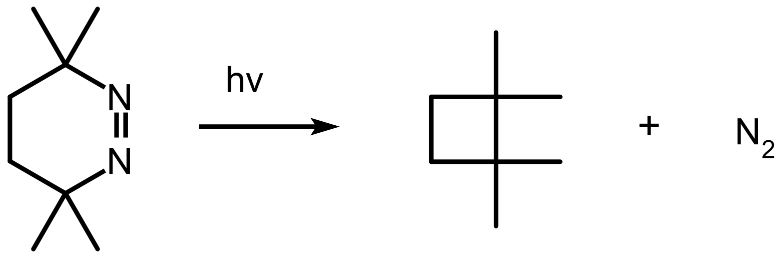
Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 153

extrusion transformation

A transformation in which an atom or group Y connected to two other atoms or groups X and Z is lost from a molecule, leading to a product in which X is bonded to Z, e.g.

$$\mathrm{X{-}Y{-}Z} \longrightarrow \mathrm{X{-}Z} + \mathrm{Y}$$

or



The reverse of an extrusion is called insertion.
See: cheletropic reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1114

f number

See: oscillator strength

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2243

f-functional branch point

Branch point from which *f* linear chains emanate.
Notes:

1. Examples are three-, four- and five-functional, branch points.
2. Alternatively, the terms trifunctional, tetrafunctional, pentafunctional, *etc*. may be used.

See also: functionality

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1818

fac-

An affix used in names to designate three groups occupying the corners of the same face of an octahedral coordination sphere, not now generally recommended for precise nomenclature purposes.

Source:
Red Book, p. 245
Blue Book, p. 464

factor

Proportionality constant between two quantities of the same dimension.

Source:
ISO 31-0: 1992 *(Quantities and Units - Part 0: General Principles, Units and Symbols.)*
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 973

fall time

See: response time

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1751

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

fallout

in atmospheric chemistry

A measurement of air contamination consisting of the mass rate at which solid particles deposit from the atmosphere.
See: dust fall

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

fanning

in atmospheric chemistry

In blast furnace operation, the idling period between the blowing periods when the blast pressure is reduced to a minimum. This also applies to plume behaviour under inversion conditions.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

farad

SI derived unit of electric capacitance, $\mathrm{F} = \mathrm{C\,V^{-1}} = \mathrm{m^{-2}\,kg^{-1}\,s^{4}\,A^{2}}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 973

faradaic current

A current corresponding to the reduction or oxidation of some chemical substance. The net faradaic current is the algebraic sum of all the faradaic currents flowing through an indicator or working electrode.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1496

faradaic current density

Measures the rate of the interfacial reaction, the proportionality constant being the charge number of the reaction multiplied by the Faraday constant.

Source:
PAC, 1980, *52*, 233 *(Electrode reaction orders, transfer coefficients and rate constants. Amplification of definitions and recommendations for publication of parameters)* on page 236

faradaic demodulation current

Component of the current that is due to the demodulation associated with an electrode reaction and that appears if an indicator or working electrode is subjected to the action of two intermodulated applied potentials of different frequency.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1496

faradaic rectification current

A component of the current that is due to the rectifying properties of an electrode reaction and that appears if an indicator or working electrode is subjected to any periodically varying applied potential while the mean value of the applied potential is controlled.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1496

Faraday constant

Fundamental physical constant representing molar elementary charge: $F = 9.648\ 533\ 99\ (24) \times 10^4\ \mathrm{C\ mol^{-1}}$.

Source:
CODATA 2006
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 973

Faraday cup (or cylinder) collector

A hollow collector, open at one end and closed at the other, used to collect beams of ions.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1553
Orange Book, p. 204

fast atom bombardment ionization

This term is used to describe ionization of any species by causing interaction of the sample (which may be dissolved in a solvent matrix) and a beam of neutral atoms having high translational energy.
See also: secondary ionization

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

fast neutrons

Neutrons of kinetic energy greater than some specified value. This value may vary over a wide range and will be dependent upon the application.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

fast-atom bombardment (FAB) mass spectroscopy

A method in which ions are produced in a mass spectrometer from non-volatile or thermally fragile organic molecules by bombarding the compound in the condensed phase with energy-rich neutral particles.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1115

fatigue

of a photochromic system

Loss of performance over time, due to chemical degradation. The major cause of fatigue is oxidation.
Note:
Although photochromism is a non-destructive process, side reactions can occur.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 338

fatty acids

Aliphatic monocarboxylic acids derived from or contained in esterified form in an animal or vegetable fat, oil or wax. Natural fatty acids commonly have a chain of 4 to 28 carbons (usually unbranched and even-numbered), which may be saturated or unsaturated. By extension, the term is sometimes used to embrace all acyclic aliphatic carboxylic acids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1335

See also:
White Book, p. 180

feed rate

in catalysis

The amount of reactant fed per unit time to the inlet of the reactor.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 82

feed-back inhibition (end product inhibition)

in biotechnology

A metabolic control mechanism in which the end product of a biochemical sequence is able to inhibit the activity of an early enzyme in the sequence, thereby controlling the metabolic flux through this pathway. As an example, isoleucine controls its own synthesis by inhibiting threonine deaminase; adenosine 5-triphosphate (ATP) and citrate control glycolysis by inhibiting phosphofructokinase.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 154

feedback

in analysis

The process whereby the output of a device is used to modify the operation of an analytical instrument.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1659

feedback

in kinetics

See: composite reaction

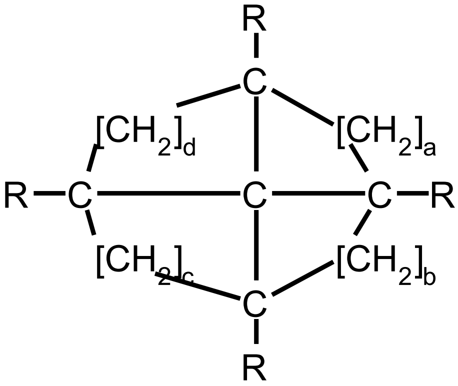
Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 166

femto

SI prefix for 10^{-15} (symbol: f).

Source:
Green Book, 2nd ed., p. 74

fenestranes



Compounds of the general formula shown above. They may be considered to be spiro compounds having bridges of carbon atoms connecting the α and α' positions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1335

Fenton reaction

$Fe^{2+} + H_2O_2 \longrightarrow Fe^{3+} + OH^{\cdot} + OH^{-}$. This is the iron-salt-dependent decomposition of dihydrogen peroxide, generating the highly reactive hydroxyl radical, possibly *via* an oxoiron(IV) intermediate. Addition of a reducing agent, such as ascorbate, leads to a cycle which increases the damage to biological molecules.
See also: Haber-Weiss reaction

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1274

fermentation

1. In metabolism, the dehydrogenating degradation of organic substance by organisms or cells under anaerobic conditions in which electrons are transferred to metabolites which accumulate and are excreted in reduced form. Fermentation is only possible if the organism is able to gain energy by this process.
2. In microbiology, the process in which cells (microorganisms, plant or animal cells) are cultured in a bioreactor in liquid or solid medium to convert organic substances into biomass (growth) or into products.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 154

fermenter

A bioreactor which enables optimal fermentation conditions to be maintained, allowing addition of nutrients, removal of products and insertion of measuring and/or control probes as well as other necessary equipment (e.g. for heating, cooling, aeration, agitation, sterilization, etc.) under sterile conditions.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 154

fermi

Non-SI unit of length, $\mathrm{f} = 10^{-15}\ \mathrm{m}$, used in nuclear physics.

Source:
Green Book, 2nd ed., p. 110

Fermi energy

The total energy of an electron in an uncharged metal at the Fermi level.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 440

Fermi level, E_F

The chemical potential of electrons in a solid (metals, semiconductors or insulators) or in an electrolyte solution.
See: bandgap energy, conduction band, valence band

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2242

See also:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 440

fermion

Particle of half-integer spin quantum number following Fermi–Dirac statistics.

Source:
Physical Chemistry Division, unpublished

ferredoxin

A protein containing more than one iron and acid-labile sulfur, that displays electron-transfer activity but not classical enzyme function.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1275

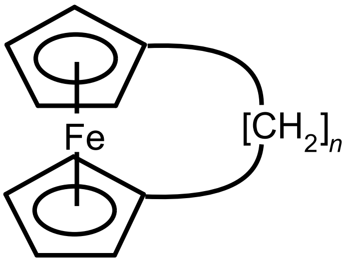
ferrimagnetic transition

See: ferroic transition, magnetic transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 582

ferrocenophanes

Compounds in which the two ring components of ferrocene are linked by one or more bridging chains.



See also: cyclophanes, metallocenes, sandwich compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1335

ferroelastic transition

A transition in which a crystal switches from one stable orientation state into another that is equally stable by the application of a mechanical stress along an appropriate direction.
See: ferroic transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 582

ferroelectric (antiferroelectric) transition

A transition from a ferroelectric to either another ferroelectric, or a paraelectric, or an antiferroelectric state. Example: The transition of the low-temperature, cubic paraelectric $BaTiO_3$ to the high-temperature, tetragonal, ferroelectric form at 393 K.
Notes:

1. In an antiferroelectric transition individual dipoles become arranged antiparallel to adjacent dipoles with the result that the net spontaneous polarization is zero.
2. Ferroelectric/antiferroelectric transitions also occur in the liquid-crystal state. These states are dependent on the alternating nature of dipoles between layers in the smectic state.

See: ferroic transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 582

ferroelectric polymer

Polymer in which spontaneous polarization arises when dipoles become arranged parallel to each other by electric fields.
Notes:

1. ***See also:*** ferroelectric transition.
2. Poly(vinylidene fluoride) after being subjected to a corona discharge is an example of a ferroelectric polymer.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 899

ferroic transition

A general term for ferroelastic, ferroelectric, antiferroelectric, ferromagnetic, antiferromagnetic and ferrimagnetic transitions in which a suitable driving force switches a ferroic crystal from one orientation state, or domain state, to another.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 582

ferromagnetic polymer

Polymer that exhibits magnetic properties because it has unpaired electron spins aligned parallel to each other or electron spins that can easily be so aligned.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 899

ferromagnetic transition

See: ferroic transition, magnetic transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 583

fertile

in radioanalytical chemistry

1. Of a nuclide: capable of being transformed, directly or indirectly, into a fissile nuclide by neutron capture.
2. Of a material: containing one or more fertile nuclides.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

fibrillar morphology

Morphology in which phase domains have shapes with one dimension much larger than the other two dimensions.
Note:
Fibrillar phase domains have the appearance of fibres.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2003

fibrous activated carbon

An activated carbon in the form of fibres, filaments, yarns or rovings and fabrics or felts. Such fibres differ from carbon fibres used for reinforcement purposes in composites by their high surface area, high porosity and low mechanical strength.
Note:
Sometimes fabrics of fibrous activated carbon are named charcoal cloths; a more precise term is 'activated carbon cloth'.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 488

fibrous carbon

See: filamentous carbon

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 488

fibrous crystal

in polymers

A type of crystal significantly longer in one dimension than in either of the other two. Fibrous crystals may comprise essentially extended chains parallel to the fibre axis; however, macroscopic polymer fibres containing chain-folded crystals are also known.

Source:
Purple Book, p. 83

fiducial group

See: helicity, torsion angle

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208

field desorption

in mass spectrometry

A term used to describe the formation of ions in the gas phase from a material deposited on a solid surface (known as an 'emitter') in the presence of a high electrical field. 'Field desorption' is an ambiguous term because it implies that the electric field desorbs a material as an ion from some kind of emitter on which the material is deposited. There is growing evidence that some of the ions formed are due to thermal ionization and some to field ionization of vapour evaporated from material on the emitter. Because there is generally little or no ionization unless the emitter is heated by an electric current, 'field desorption' is a misnomer. The term is, however, firmly implanted in the literature and most users undertand what is going on regardless of the implications of the term. In addition, no better simple term has been suggested to take its place and so, reluctantly, it is recommended that it be retained.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

field effect

Also contains definition of: direct effect

An experimentally observable effect symbolized by F (on reaction rates, etc.) of intramolecular coulombic interaction between the centre of interest and a remote unipole or dipole, by direct action through space rather than through bonds. The magnitude of the field effect (or 'direct effect') depends on the unipolar charge/dipole moment, orientation of dipole, shortest distance between the centre of interest and the remote unipole or dipole, and on the effective dielectric constant.
See also: electronic effect, inductive effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1115

field ionization

in mass spectrometry

The removal of electrons from any species by interaction with a high electrical field.
See also: field desorption

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548
Orange Book, p. 203

field level

Logarithm of the ratio of two values of a field quantity, usually amplitude. Levels are expressed in different ways: $L_F = \ln\left(\frac{F}{F_0}\right) N_{\mathrm{p}}$, where N_{p} is the symbol for the unit neper coherent with the SI, or $L_F = 20 \log_{10}\left(\frac{F}{F_0}\right) \mathrm{dB}$, where dB is the symbol for the unit decibel.

Source:
Green Book, 2nd ed., p. 79

filamentous carbon

A carbonaceous deposit from gaseous carbon compounds, consisting of filaments grown by the catalytic action of metal particles.
Note:
In general, such deposits are obtained at pressures of $< \mathrm{kPa}$ in the temperature region 600 - $1300\ \mathrm{K}$ on metals such as iron, cobalt or nickel. Typical filaments consist of a duplex structure, a relatively oxidation-resistant skin surrounding a more easily oxidizable core, with a metal particle located at the growing end of the filament. They generally range from 0.01 to $0.5\ \mu\mathrm{m}$ in diameter and up to $10\ \mu\mathrm{m}$ in length. In some systems, the metal particles are located in the middle of the filaments, and there are also examples where several filaments originate from a single particle. The filaments may be produced in different conformations, such as helical, twisted and straight.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 488

filler

Also contains definition of: grist

Filler (also called grist) is a petroleum- or coal-based coke fraction of a green, carbon mix or formulation. Coarse particles, $> 0.425\ \mathrm{mm}$, are sometimes referred to as tailings; fine particles, $< 0.074\ \mathrm{mm}$, are referred to as flour. Graphite flour is also used as a filler.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 489

filler coke

The main constituent of a carbon artifact, introduced as solid component (predominantly in the form of particulate carbon) into the 'carbon mix' from which polygranular carbon and graphite materials are obtained by heat treatment.
Note:
Filler coke is not necessarily the only, but it is commonly the most important filler material used in a 'carbon mix' which consists of filler and binder.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 489

filling solution

of a reference electrode

Solution containing the anion to which the reference electrode of the operational pH cell is reversible, e.g. chloride for silver-silver chloride electrode. In the absence of a bridge solution, a high concentration of filling solution comprising cations and anions of almost equal mobility is employed as a means of maintaining the liquid junction potential small and approximately constant on substitution of test solution for standard solution(s).

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 541

film

A generic term referring to condensed matter restricted in one dimension.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1671

film badge

in radioanalytical chemistry

A package containing one or more small photographic films for approximate measurement of radiation exposure, used for the purpose of monitoring personnel.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

film element

A small homogeneous part of a film including the two interfaces and any fluid between them.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

film tension

The contractile force per unit length, Σ_{f}, exerted by an equilibrium film in contact with the bulk phase.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 614

filter

A porous material on which solid particles present in air or other fluid which flows through it are largely caught and retained. Filters are made with a variety of materials: cellulose and derivatives, glass fibre, ceramic, synthetic plastics and fibres. Filters may be naturally porous or be made so by mechanical or other means. Membrane/ceramic filters are prepared with highly controlled pore size in a sheet of suitable material such as polyfluoroethylene, polycarbonate or cellulose esters. Nylon mesh is sometimes used for reinforcement. The pores constitute 80–85% of the filter volume commonly and several pore sizes are available for air sampling ($0.45 - 0.8\ \mu\mathrm{m}$ are commonly employed).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

filter

of a radiation

Material interposed in the path of radiation to modify the spectral distribution of the radiation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2519

filter spectrometer

A spectrometer which has one or more spectral filters for isolating one or more spectral bands.

Source:
PAC, 1995, *67*, 1725 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-IX. Instrumentation for the spectral dispersion and isolation of optical radiation (IUPAC Recommendations 1995))* on page 1729

filtration

The process of segregation of phases; e.g. the separation of suspended solids from a liquid or gas, usually by forcing a carrier gas or liquid through a porous medium.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

fine structure constant, α

Atomic fundamental physical constant, $\alpha = \frac{\mu_0 \, e^2 \, c_0}{2 \, h} = 7.297\,353\,08\,(33) \times 10^{-3}$, where μ_0 is the permeability of vacuum, e the elementary charge, h the Planck constant, and c_0 the speed of light.

Source:
CODATA Bull. 1986, *63*, 1

first-order phase transition

Synonym: discontinuous phase transition

A transition in which the molar Gibbs energies or molar Helmholtz energies of the two phases (or chemical potentials of all components in the two phases) are equal at the transition temperature, but their first derivatives with respect to temperature and pressure (for example, specific enthalpy of transition and specific volume) are discontinuous at the transition point, as for two dissimilar phases that coexist and that can be transformed into one another by a change in a field variable such as pressure, temperature, magnetic or electric field. Example: The transition on heating CsCl to $752\ \mathrm{K}$ at which it changes from the low-temperature, CsCl-type structure to the high-temperature NaCl-type structure. Synonymous with discontinuous phase transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 583

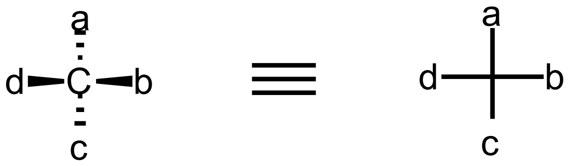
first-pass effect

Biotransformation and, in some cases, elimination of a substance in the liver after absorption from the intestine and before it reaches the systemic circulation.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1052

Fischer projection (Fischer–Tollens projection)

A projection formula in which vertically drawn bonds are considered to lie below the projection plane and horizontal bonds to lie above that plane. Thus for the molecule Cabcd:

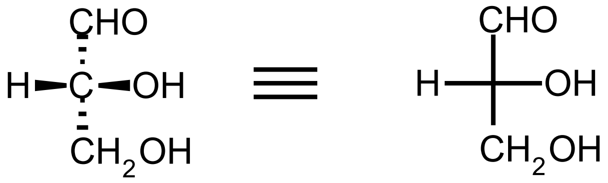


Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208
Blue Book, p. 484

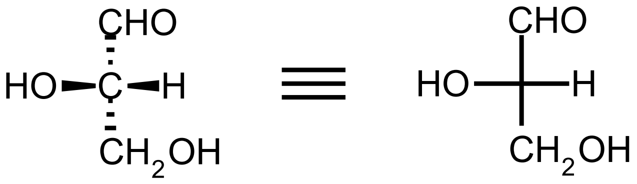
See also:
White Book, p. 128

Fischer–Rosanoff convention (or Rosanoff convention)

An arbitrary convention according to which (+)-glyceraldehyde, now known to be (*R*)-2,3-dihydroxypropanal, was named D-glyceraldehyde (with the enantiomer L-glyceraldehyde and its racemate DL-glyceraldehyde) and taken to have the absolute configuration represented by the Fischer projection formula shown in the diagram.



D-glyceraldehyde



L-glyceraldehyde

The atom numbered 1 according to normal nomenclature rules is conventionally placed at the top of the main chain, which is drawn vertically and other groups are drawn on either side of that main chain. The convention is still in use for α-amino acids and for sugars.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2208

fissile

in radioanalytical chemistry

1. Of a nuclide: capable of undergoing fission by interaction with (slow) neutrons.
2. Of a material: containing one or more fissile nuclides.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

fission fragment ionization

in mass spectrometry

See: plasma desorption ionization

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548

fission fragments

Nuclei resulting from fission and possessing kinetic energy acquired from the fission process.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

fission neutrons

Neutrons originating in the fission process which have retained their original energy.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

fission products

Nuclides produced by fission and the daughter products of these nuclides.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

fission yield

The fraction of fissions leading to fission products of a given type.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

fissionable

Synonymous with fissile.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

fixed ions

In an ion exchanger, the non-exchangeable ions which have a charge opposite to that of the counter-ions.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 854

fixed neutral loss (gain) scan

in mass spectrometry

A scan which determines, in a single experiment, all the parent ion mass-to-charge ratios which react to the loss or gain of a selected neutral mass.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1551

fixed neutral loss (gain) spectrum

in mass spectrometry

A spectrum obtained when data are acquired that determine all the parent ion mass-to-charge ratios that react by the loss (gain) of a selected neutral mass.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1551

fixed precursor ion scan

in mass spectrometry

A scan which determines, in a single experiment, all the daughter ion mass-to-charge ratios that are produced by the reaction of a selected parent ion mass-to-charge ratio.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1551

fixed product ion scan

in mass spectrometry

A scan which determines, in a single experiment, all the parent ion mass-to-charge ratios that react to produce a selected daughter ion mass-to-charge ratio (sometimes called a 'parent ion scan').

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1551

fixed product ion spectrum

in mass spectrometry

A spectrum obtained when data are acquired that determine all the parent ion mass-to-charge ratios that react to produce a selected daughter ion mass-to-charge ratio.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1551

flame ionization detector

in gas chromatography

The gases emerging from the column are fed into a hydrogen flame across which an electrical potential is placed. Certain molecules ionize easily in the flame and the current produced is proportional to the instantaneous flow rate of the eluted component. The detector is relatively insensitive to inorganic molecules and is most used for organic compounds. Concentrations below $1\ \mathrm{ppmv}$ are easily detected. The linear dynamic range is between 10^3 and 10^5.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

flame photometric detector

in gas chromatography

The eluent from the column is fed into a hydrogen-rich flame and produces light emission. Optical filters are used to select the wavelength range of the emission which is characteristic of specific atoms (usually sulfur or phosphorus). The detector is very specific, depending on the choice of optical filters. It can detect the S- and P-containing compounds down to $10^{-3}\ \mathrm{ppmv}$, but the detector is non-linear.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

flame photometry

The use of emission spectroscopy in the ultraviolet and visible regions to identify and estimate the amounts of various elements which are excited in a flame, an arc or high voltage spark.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

flame-in-tube atomizer

in spectrochemical analysis

An atomizer in which hydrogen, used as carrier gas, is partially combusted in the inlet arm of a T-shaped tube furnace by introducing a limited amount of oxygen or air.

Source:
PAC, 1992, *64*, 261 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XIII. Terms related to chemical vapour generation (IUPAC Recommendations 1992))* on page 264

flammable limits

See: explosivity limits

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

flash fluorimetry (phosphorimetry)

The term used when decay times luminescence are measured using a pulsed source of radiation. It is often necessary to separate the signal due to the light flash from luminescence emission signal by a deconvolution technique in order to obtain the correct decay curve for emission. Decay times corrected for this effect are termed corrected decay times of fluorescence or phosphorescence.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 242

flash lamps

Lamps which contain an inert gas which can be rapidly pulsed.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 238

flash photolysis

A technique of transient spectroscopy and transient kinetic studies in which a light pulse is used to produce transient species. Commonly, an intense pulse of short duration is used to produce a sufficient concentration of a transient species suitable for spectroscopic observation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2242

flash point

The lowest temperature at which a substance, e.g. fuel oil, will give off a vapour that will flash or burn momentarily when ignited.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

flash vacuum pyrolysis (FVP)

Thermal reaction of a molecule by exposing it to a short thermal shock at high temperature, usually in the gas phase.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1115
PAC, 1993, *65*, 2405 *(Nomenclature and terminology for analytical pyrolysis (IUPAC Recommendations 1993))* on page 2407

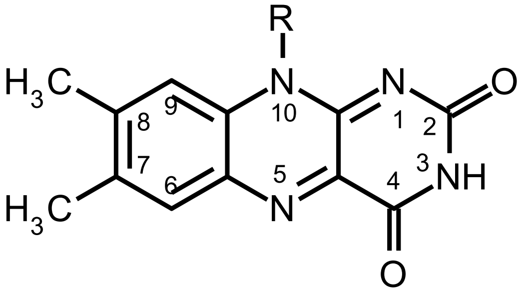
flat band potential (at a semiconductor/solution interphase)

If effects of surface states are negligible, $\Delta\varphi^{\mathrm{sc}}$, the potential drop associated with the space charge in the semiconductor, vanishes as the charge on the semiconductor becomes zero. The potential of the semiconductor corresponding to this condition is the flat band potential, which plays the same role as the potential of zero charge for metals.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 444

flavins

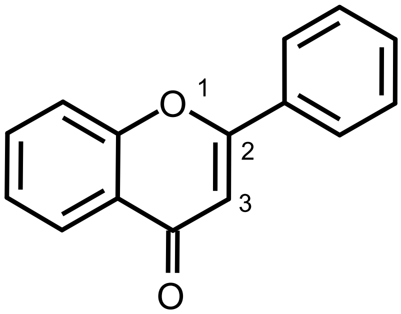
Derivatives of the dimethylisoalloxazine (7,8-dimethylbenzo[*g*]pteridine- 2,4(3*H*,10*H*)-dione) skeleton, with a substituent on the 10 position. (Riboflavin, having a 10-D-ribityl group, is the most prominent member).



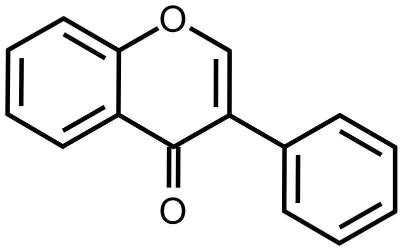
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1335

flavonoids (isoflavonoids and neoflavonoids)

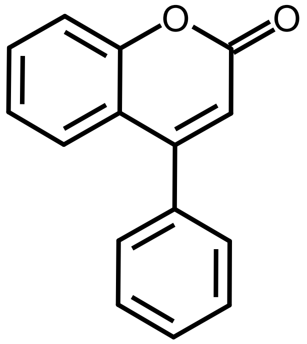
Flavonoids, isoflavonoids and neoflavonoids are natural products derived from 2-phenylchromen-4-one (flavone), 3-phenylchromen-4-one and 4-phenylcoumarin, respectively. Derivations include reduction of the 2(3) carbon-carbon double bond (flavanones), reduction of the keto group (flavanols), and hydroxylation at various positions.



2-phenylchromen-4-one



3-phenylchromen-4-one



4-phenylcoumarin

See also: anthocyanins, chalcones

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1335

flavoproteins

Flavins tightly bound or covalently attached to a protein chain, commonly through the 8-methyl carbon atom.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1335

floc

When a sol is colloidally unstable the formation of aggregates is called coagulation or flocculation. Some authors distinguish between coagulation and flocculation, the latter implying the formation of a loose or open network which may or may not separate macroscopically. The loose structure formed in this way is called a floc.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

floccule

A small loosely aggregated mass of material suspended in or precipitated from a liquid; a cluster of particles.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

Flory–Huggins theory

A thermodynamic theory of polymer solutions, first formulated independently by Flory and by Huggins, in which the thermodynamic quantities of the solution are derived from a simple concept of combinatorial entropy of mixing and a reduced Gibbs energy parameter, the 'χ parameter'.

Source:
Purple Book, p. 59

flotation

The removal of matter by entrainment at an interface.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 609

flow analysis

The generic name for all analytical methods that are based on the introduction and processing of test samples in flowing media.

Source:
PAC, 1994, *66*, 2493 *(Classification and definition of analytical methods based on flowing media (IUPAC Recommendations 1994))* on page 2496
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2189

flow enthalpimetry [obsolete]

See: flow injection enthalpimetry

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2491

flow injection

The introduction of a sample or reagent into a continuous stream by use of a rapid delivery device.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

flow injection enthalpimetry

Synonym: enthalpimetric flow injection analysis

A term used to describe several related methods in which a transient temperature change in a flowing liquid stream, caused by a chemical reaction, is used to quantitatively determine an analyte. The analyte is introduced as a discrete liquid sample (i.e. test portion) into the flowing stream. This definition limits the scope to experiments with primarily an analytical emphasis, performed in a flow injection calorimeter. This maintains a clear distinction from classical flow calorimetric methods where reagents are combined continuously in flowing streams, or where the heat effect is measured *via* the flowing of a fluid over a reaction vessel. An acceptable synonym is enthalpimetric flow injection analysis. Other non-recommended terms which have been used in the literature include peak enthalpimetry and enzyme thermistor. Flow enthalpimetry has been used to describe the flow injection technique, but its use for this purpose is discouraged.

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2491

flow rate

in chromatography

The volume of mobile phase passing through the column in unit time. The flow rate is usually measured at column outlet, at ambient pressure (p_a) and temperature (T_a, in K); this value is indicated with the symbol F. If a water-containing flowmeter was used for the measurement (e.g. the so-called soap bubble flowmeter) then F must be corrected to dry gas conditions in order to obtain the mobile phase flow rate at ambient temperature (F_a):

$$F_a = F\left(1 - \frac{p_w}{p_a}\right)$$

where p_w is the partial pressure of water vapour at ambient temperature. In order to specify chromatographic conditions in column chromatography, the flow-rate (mobile phase flow rate at column temperature, F_c) must be expressed at T_c (kelvin), the column temperature:

$$F_c = F_a \frac{T_c}{T_a}$$

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 839

flow rate

in flame emission and absorption spectrometry

The volume rate of one component, **X** (e.g. air, O_2), of the unburnt gas mixture (such as C_2H_2, O_2, etc.) in the burner tip. Ambient temperature and pressure must be stated.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1742

flow rate

of a quantity

Quantity X (e.g. heat, amount, mass, volume, ...) transferred in a time interval divided by that time interval. General symbols: q_X, $\dot{X}$.

Source:
Green Book, 2nd ed., p. 65

flow rate of unburnt gas mixture

in flame emission and absorption spectrometry

The volume rate of the gas mixture of the burner tip. It depends on operating conditions such as gas pressure; the ambient temperature and pressure should also be stated.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1742

flow reactor

A reactor through which the reactants pass while catalysis is in progress.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

flow resistance parameter, Φ

in chromatography

A term used to compare packing density and permeability of columns packed with different particles; it is dimensionless.

$$\Phi = \frac{{d_\mathrm{p}}^2}{B_0}$$

where d_p is the average particle diameter. In open-tubular columns $\Phi = 32$.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 833

flow-programmed chromatography

A procedure in which the rate of flow of the mobile phase is changed systematically during a part or the whole of the separation.

Source:
Orange Book, p. 92

flue gas

in atmospheric chemistry

Waste gas from the combustion process.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2189

flue gas scrubber

in atmospheric chemistry

Equipment for removing fly ash and other objectionable materials from the products of combustion by means of sprays or wet baffles.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2189

fluence, F, Ψ, H_0

At a given point in space, the radiant energy incident on a small sphere divided by the cross-sectional area of that sphere. It is used in photochemistry to specify the energy delivered in a given time interval (for instance by a laser pulse).
See also: dose, photon fluence

Source:
Green Book, 2nd ed., p. 31
ISO 31-5: 1992 *(Quantities and Units - Part 5: Electricity and Magnetism.)*

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2242

fluence rate, E_o

Also contains definitions of: radiant energy fluence rate, spherical irradiance

Total radiant power, P, incident from all directions onto a small sphere divided by the cross-sectional area of that sphere. SI unit is $\mathrm{W\ m^{-2}}$.
Notes:

1. Mathematical definition: $E_\mathrm{o} = \frac{\mathrm{d}P}{\mathrm{d}S} = \frac{\mathrm{d}H_\mathrm{o}}{\mathrm{d}t}$. If the radiant power is constant over the area S, $E_\mathrm{o} = \frac{P}{S}$. Equivalent definition: $E_\mathrm{o} = \int_{4\pi} L\mathrm{d}\Omega$, with Ω the solid angle of each beam passing through the given point on the surface and L the radiance of the beam at that point.
2. Fluence rate is identical to spherical irradiance and reduces to irradiance, E, for a parallel and perpendicularly incident beam not scattered or reflected by the target or its surroundings.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 340

fluid coke

The carbonization product of high-boiling hydrocarbon fractions (heavy residues of petroleum or coal processing) produced by the fluid coking process.
Note:
Fluid coke consists of spherulitic grains with a spherical layer structure and is generally less graphitizable than delayed coke. Therefore, it is not suitable as filler coke for polygranular graphite products and is also less suitable for polycrystalline carbon products. Because of its isotropy it is less suitable to produce an anisotropic synthetic graphite. All cokes contain a fraction of matter that can

be released as volatiles during heat treatment. This mass fraction, the so-called volatile matter, is in the case of fluid coke about 6 wt.%.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 489

fluidity, ϕ

Reciprocal of dynamic viscosity.

Source:
Green Book, 2nd ed., p. 13

fluidized bed

A catalyst bed in which the flow of gases is sufficient to cause the finely divided particles to behave like a fluid.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

fluoresceins

See: xanthene dyes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

fluorescence

Luminescence which occurs essentially only during the irradiation of a substance by electromagnetic radiation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2519
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 233

fluorescence error

in spectrochemical analysis

Some samples are excited to fluorescence by the incident radiation beam. When added to the transmitted radiation beam this fluorescence results in an erroneous reading called the fluorescence error. It is particularly noticeable if the photodetector is situated close to the sample.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1457

fluorescence lifetime

Parameter describing the time evolution of the decay of the fluorescent radiant intensity.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 340

fluorescence resonance energy transfer

Term frequently and inappropriately applied to resonance energy transfer in the sense of Förster-resonance-energy transfer (FRET), which does not involve the emission of radiation.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 340

fluorescence yield

For a given transition from an excited state of a specified atom, the ratio of the number of excited atoms which emit a photon to the total number of excited atoms.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

See also:
Orange Book, p. 174

fluorimeter

An instrument used to measure the intensity and the wavelength distribution of the light emitted as fluorescence from a molecule excited at a specific wavelength or wavelengths within the absorption band of a particular compound. Characteristic fluorescence bands may be used to identify specific pollutants such as the polynuclear aromatic hydrocarbons. Excitation spectra of impurities can be observed by scanning the wavelength of the excitation light which is incident on the sample over a range of wavelengths and observing the relative intensity of the fluorescence emitted at a given wavelength. These spectra are also characteristic of the impurity.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2189

fluorocarbons

Compounds consisting wholly of fluorine and carbon.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

fluorogenic

Property of a material in which fluorescence is induced or enhanced by the addition of another molecular entity.
Note:
An example is a non-fluorescent compound consisting of a pyrene connected to a maleimide group (which quenches the pyrene fluorescence). A reaction in which the maleimide moiety is converted to a succinimide derivative results in the recovery of the pyrene fluorescence.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 341

fluorohydrins

See: halohydrins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

fluorophore

Molecular entity (often organic) that emits fluorescence.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 341

flux depression

The lowering of the particle (or photon) flux density in the neighbourhood of an object due to absorption of particles (or photons) in the object.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2519

flux, J_X

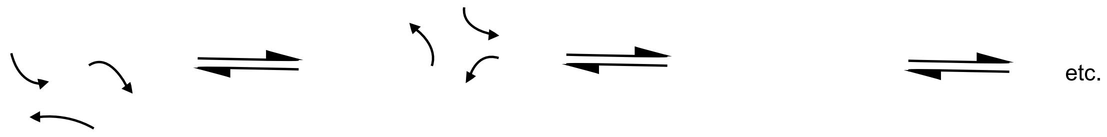
of a quantity

Flow rate of **X** through a cross-section perpendicular to the flow divided by the cross-sectional area.

Source:
Green Book, 2nd ed., p. 65
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 974

fluxional

A chemical species is said to be fluxional if it undergoes rapid degenerate rearrangements (generally detectable by methods which allow the observation of the behaviour of individual nuclei in a rearranged chemical species, e.g. NMR, X-ray). Example: bullvalene (1 209 600 interconvertible arrangements of the ten CH groups).



The term is also used to designate positional change among ligands of complex compounds and organometallics. In these cases, the change is not necessarily degenerate.
See also: valence tautomerization

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1115

fly ash

in atmospheric chemistry

Finely divided particles of ash entrained in flue gases resulting from the combustion of fuel.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2190

foam

A dispersion in which a large proportion of gas by volume in the form of gas bubbles, is dispersed in a liquid, solid or gel. The diameter of the bubbles is usually larger than $1\ \mu m$, but the thickness of the lamellae between the bubbles is often in the usual colloidal size range. The term froth has been used interchangeably with foam. In particular cases froth may be distinguished from foam by the fact that the former is stabilized by solid particles (as in froth flotation q.v.) and the latter by soluble substances.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 606

foam fractionation

A method of separation in which a component of the bulk liquid is preferentially adsorbed at the liquid/vapour (L/V) interface and is removed by foaming.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 609

foaming agent

A surfactant which when present in small amounts facilitates the formation of a foam, or enhances its colloidal stability by inhibiting the coalescence of bubbles.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

fog

A general term applied to a suspension of droplets in a gas. In meteorology, it refers to a suspension of water droplets resulting in a visibility of less than $1\ km$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2190
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 606

fog horizon

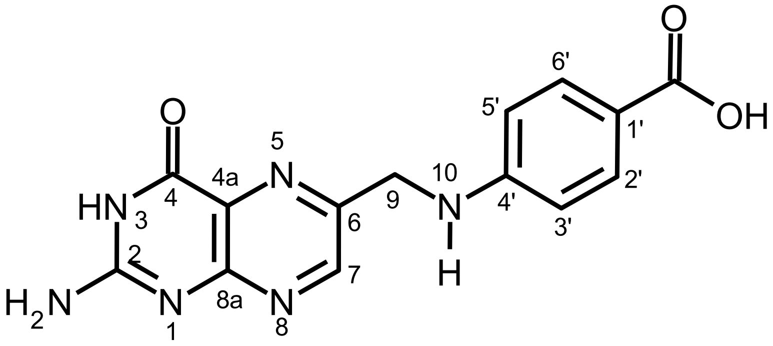
in atmospheric chemistry

The top of a fog layer which is confined by a low-level temperature inversion and gives the appearance of the horizon (which it actually obscures) when viewed from above, against the sky.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2190

folates

A group of heterocyclic compounds based on the pteroic acid skeleton (below) conjugated with one or more L-glutamate units.



Source:
White Book, p. 266

fold domain

in polymer crystals

A portion of a polymer crystal wherein the fold planes have the same orientation. The sectors of lamellar crystals frequently represent fold domains.

Source:
Purple Book, p. 83

fold

in polymer crystals

The loop connecting two different stems in a folded chain.

Source:
Purple Book, p. 83

fold plane

in polymer crystals

A crystallographic plane defined by a large number of stems that are connected by chain folds.

Source:
Purple Book, p. 83

fold surface

in polymer crystals

A surface approximately tangential to the folds.

Source:
Purple Book, p. 83

folded-chain crystal

in polymers

A polymer crystal consisting predominantly of chains that traverse the crystal repeatedly by folding as they emerge at its external surfaces. The re-entry of the chain into the crystal is assumed to be adjacent or near-adjacent within the lattice.

Source:
Purple Book, p. 84

foot

Non-SI unit of length, $\mathrm{ft} = 12\ \mathrm{in} = 0.3048\ \mathrm{m}$.

Source:
Green Book, 2nd ed., p. 110

forbidden line

in X-ray spectroscopy

See: selection rule

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 738

force, F

Derivative of momentum with respect to time.

Source:
Green Book, 2nd ed., p. 12
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 974

force constants

The coefficients in an expansion of the intramolecular potential function in terms of a definite set of coordinates, the values of which define the deformation of the molecule away from its equilibrium configuration. In order to define force constants, one has to indicate both the definition of each coordinate and the expansion of the potential.

Source:
PAC, 1978, *50*, 1707 *(Definition and symbolism of molecular force constants)* on page 1709

formamidine disulfides

The compound $H_2NC(=NH)SSC(=NH)NH_2$ and its derivatives formed by substitution at nitrogen.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

formation constant

For a mononuclear binary complex, if a central atom (central group) M (the 'metal') and a ligand L have been defined, then in the following expressions K_n is the stepwise formation constant, and β_n is the cumulative formation constant for the complex ML_n. They can both be referred to as stability constants (stepwise and cumulative).

$$K_n = K(\mathrm{ML}_{n-1} + \mathrm{L} \rightleftharpoons \mathrm{ML}_n)$$

$$\beta_n = K(\mathrm{M} + n\,\mathrm{L} \rightleftharpoons \mathrm{ML}_n)$$

Source:
Orange Book, p. 11

formazans

The parent compound $H_2NN=CHN=NH$ and its derivatives formed by substitution at carbon and/or nitrogen.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

Förster cycle

An indirect method of determination of excited state equilibria, such as $\mathrm{p}K^{*,\mathrm{a}}$ values, based on ground state thermodynamics and electronic transition energies. This cycle considers only the difference in molar enthalpy change ($\Delta\Delta H$) of reaction of ground and excited states, neglecting the difference in molar entropy change of reaction of those states ($\Delta\Delta S$).

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2243

Förster excitation transfer (dipole–dipole excitation transfer)

Also contains definition of: critical quenching radius, r_0

A mechanism of excitation transfer which can occur between molecular entities separated by distances considerably exceeding the sum of their van der Waals radii. It is described in terms of an interaction between the transition dipole moments (a dipolar mechanism). The transfer rate constant $k_{\mathrm{D} \rightarrow \mathrm{A}}$ is given by:

$$k_{\mathrm{D} \rightarrow \mathrm{A}} = \frac{K^2\, J\, 8.8 \times 10^{-28}\,\mathrm{mol}}{n^4\, \tau_0\, r^6}$$

where K is an orientation factor, n the refractive index of the medium, τ_0 the radiative lifetime of the donor, r the distance (cm) between donor (D) and acceptor (A), and J the spectral overlap (in coherent units $\mathrm{cm}^6\ \mathrm{mol}^{-1}$) between the absorption spectrum of the acceptor and the fluorescence spectrum of the donor. The critical quenching radius, r_0, is that distance at which $k_{\mathrm{D} \rightarrow \mathrm{A}}$ is equal to the inverse of the radiative lifetime.
See also: Dexter excitation transfer, energy transfer, radiative energy transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2243

Förster-resonance-energy transfer FRET

Also contains definition of: dipole–dipole excitation transfer

Non-radiative excitation transfer between two molecular entities separated by distances considerably exceeding the sum of their van der Waals radii. It describes the transfer in terms of the interaction between the transition (dipole) moments of the entities in the very weak dipole-dipole coupling limit. It is a Coulombic interaction frequently called a dipole-dipole coupling. The transfer rate constant from donor to acceptor, k_{T}, is given by

$$k_{\mathrm{T}} = k_{\mathrm{D}} \left(\frac{R_0}{r}\right)^6 = \frac{1}{\tau_{\mathrm{D}}^0} \left(\frac{R_0}{r}\right)^6$$

where k_{D} and τ_{D}^0 are the emission rate constant and the lifetime of the excited donor in the absence of transfer, respectively, r is the distance between the donor and the acceptor and R_0 is the critical quenching radius or Förster radius, i.e., the distance at which transfer and spontaneous decay of the excited donor are equally probable ($k_{\mathrm{T}} = k_{\mathrm{D}}$) (see Note 3).

R_0 is given by

$$R_0 = Const. \left(\frac{\kappa^2\, \Phi_{\mathrm{D}}^0\, J}{n^4}\right)^{1/6}$$

where κ is the orientation factor, Φ_{D}^{0} is the fluorescence quantum yield of the donor in the absence of transfer, n is the average refractive index of the medium in the wavelength range where spectral overlap is significant, J is the spectral overlap integral reflecting the degree of overlap of the donor emission spectrum with the acceptor absorption spectrum and given by

$$J = \int_{\lambda} I_{\lambda}^{\mathrm{D}}(\lambda)\,\varepsilon_{\mathrm{A}}(\lambda)\,\lambda^{4}\mathrm{d}\lambda$$

where $I_{\lambda}^{\mathrm{D}}(\lambda)$ is the normalized spectral radiant intensity of the donor so that $\int_{\lambda} I_{\lambda}^{\mathrm{D}}(\lambda)\mathrm{d}\lambda = 1$. $\varepsilon_{\mathrm{A}}(\lambda)$ is the molar decadic absorption coefficient of the acceptor. See Note 3 for the value of $Const.$.

Notes:

1. The bandpass $\Delta\lambda$ is a constant in spectrophotometers and spectrofluorometers using gratings. Thus, the scale is linear in wavelength and it is convenient to express and calculate the integrals in wavelengths instead of wavenumbers in order to avoid confusion.
2. In practical terms, the integral $\int_{\lambda} I_{\lambda}^{\mathrm{D}}(\lambda)\mathrm{d}\lambda$ is the area under the plot of the donor emission intensity versus the emission wavelength.
3. A practical expression for R_0 is:

$$\frac{R_0}{\mathrm{nm}} = 2.108 \times 10^{-2} \left\{\kappa^{2}\,\Phi_{\mathrm{D}}^{0}\,n^{-4} \int_{\lambda} I_{\lambda}^{\mathrm{D}}(\lambda) \left[\frac{\varepsilon_{\mathrm{A}}(\lambda)}{\mathrm{dm}^{3}\ \mathrm{mol}^{-1}\ \mathrm{cm}^{-1}}\right] \left(\frac{\lambda}{\mathrm{nm}}\right)^{4} \mathrm{d}\lambda \right\}^{1/6}$$

   The orientation factor κ is given by

$$\kappa = \cos\theta_{\mathrm{DA}} - 3\cos\theta_{\mathrm{D}}\cos\theta_{\mathrm{A}} = \sin\theta_{\mathrm{D}}\sin\theta_{\mathrm{A}}\cos\varphi - 2\cos\theta_{\mathrm{D}}\cos\theta_{\mathrm{A}}$$

   where θ_{DA} is the angle between the donor and acceptor moments, and θ_{D} and θ_{A} are the angles between these, respectively, and the separation vector; φ is the angle between the projections of the transition moments on a plane perpendicular to the line through the centres. κ^{2} can in principle take values from 0 (perpendicular transition moments) to 4 (collinear transition moments). When the transition moments are parallel and perpendicular to the separation vector, $\kappa^{2} = 1$. When they are in line (i.e., their moments are strictly along the separation vector), $\kappa^{2} = 4$. For randomly oriented transition (dipole) moments, e.g., in fluid solutions, $\kappa^{2} = \frac{2}{3}$.
4. The transfer quantum efficiency is defined as

$$\Phi_{\mathrm{T}} = \frac{k_{\mathrm{T}}}{k_{\mathrm{D}} + k_{\mathrm{T}}}$$

   and can be related to the ratio $\frac{r}{R_0}$ as follows:

$$\Phi_{\mathrm{T}} = \frac{1}{1 + (\frac{r}{R_0})^6}$$

or written in the following form :

$$\Phi_{\mathrm{T}} = 1 - \frac{\tau_{\mathrm{D}}}{\tau_{\mathrm{D}}^0}$$

where τ_{D} is the donor excited-state lifetime in the presence of acceptor, and τ_{D}^0 in the absence of acceptor.

5. FRET is sometimes inappropriately called fluorescence-resonance energy transfer. This is not correct because there is no fluorescence involved in FRET.
6. Foerster is an alternative and acceptable spelling for Förster.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 342

fossil fuel

A fuel such as coal, oil and natural gas which has formed over many years through the decomposition of deposited vegetation which was under extreme pressure of an overburden of earth.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2190

fouling agent

Synonym: mechanical inhibitor *in catalysis*

in catalysis

Fouling agents (or mechanical inhibitors) are inhibitory substances bound by neither covalent nor other strong bonds to the active centres: the interaction is usually of the van der Waals, H-bond or sometimes ionic, type. They form protective layers or block pores, thus physically impeding access of reactants to the active centres. The fouling agents which cause real problems are those which have a long standing effect and do not disappear spontaneously. Carbon deposits act, partially or totally, this way (see coking). Other examples are vanadium and nickel sulfide deposits in hydrotreating catalysts.

Source:
PAC, 1991, *63*, 1227 *(Manual on catalyst characterization (Recommendations 1991))* on page 1244

fouling

in membrane processes

Process resulting in loss of performance of a membrane due to the deposition of suspended or dissolved substances on its external surfaces, at its pore openings, or within its pores.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1482

Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometer

A high-frequency mass spectrometer in which the cyclotron motion of ions, having different mass/charge ratios, in a constant magnetic field is excited essentially simultaneously and coherently by a pulse or a radio-frequency electric field applied perpendicular to the magnetic field. The excited cyclotron motion of the ions is subsequently detected on so-called receiver plates as a time domain signal that contains all the cyclotron frequencies that have been excited. Fourier transformation of the time domain signal results in the frequency domain FT-ICR signal which, on the basis of the inverse proportionality between frequency and the mass/charge ratio, can be converted into a mass spectrum. The term is sometimes contracted to Fourier transform mass spectrometer (FT-MS).
See also: ion cyclotron resonance (ICR) mass spectrometer

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545

Fourier transform spectrometer

A scanning interferometer, containing no principal dispersive element, which first splits a beam into two or more components, then recombines these with a phase difference. The spectrum is obtained by a Fourier transformation of the output of the interferometer.
See also: multiplex spectrometer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2243

Fourier-transform spectroscopy

Measurement technique whereby spectra are collected based on measurements of the temporal coherence of a radiative source, using time-domain measurements of the electromagnetic radiation or other type of radiation.
Note: This procedure can be applied to a variety of spectroscopies including optical-, infrared- (FTIR), nuclear magnetic resonance-, and electron spin-resonance spectroscopy. There are several methods for measuring the temporal coherence of the light, including the CW Michelson or Fourier-transform spectrometer and the pulsed Fourier-transform spectrograph (which is more sensitive and has a much shorter sampling time than conventional spectroscopic techniques).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 344

fractal agglomerate

Agglomerate having the same fractal dimension as the constituent particles.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1811

fractal dimension, *d*

Also contains definitions of: Hausdorff dimension, mass fractal dimension

Also contains definition of: surface fractal dimension

Parameter that provides a mathematical description of the fractal structure of a polymer network, an aggregated particulate sol, or of the particles that comprise them.
Notes:

1. $m \propto r^d$ in which m is the mass contained within a radius, r, measured from any site or bond within a fractal structure.
2. For a Euclidean object of constant density, $d = 3$, but for a fractal object, $d < 3$, such that its density decreases as the object gets larger.
3. For the surface area of a fractal object, $s \propto r^{d'}$ in which s is the surface area contained within a radius, r, measured from any site or bond and d' is termed the surface fractal dimension.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1811

fraction

In general, a ratio of two quantities of the same kind, the numerator quantity applying to one constituent (or part) of the system and the denominator to the sum of quantities for all constituents (parts) of the system. When applied to mixtures fractions represent a group of 3 quantities: mass fraction, volume fraction, and amount fraction (or mole fraction equal to the number fraction).

Source:
Green Book, 2nd ed., p. 41
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 974

fraction collector
in chromatography

A device for recovering fractional volumes of the column effluent.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 829

fraction extracted, E

The fraction of the total quantity of a substance extracted (usually by the solvent) under specified conditions, i.e. $E_A = \frac{Q_A}{Q_A'}$ where Q_A is the mass of **A** extracted and Q_A' is the total mass of **A** present at the start.

Notes:

1. E may be expressed as a percentage, $\% E$.
2. The term extractability is qualitative and should not be used as a synonym for fraction extracted.
3. If the aqueous phase is extracted with n successive portions of solvent, the phase volume ratio (solvent/feed) being r each time, the fraction extracted is given by:

   $$E_n = 1 - (r\,D + 1)^{-n}$$

   If $n = r = 1$ and $E_1 = \frac{D}{1+D}$ this expression is a concept of value in chromatography theory.
4. The fraction extracted is also known as the recovery factor, especially for a multistage process.

Source:

PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2384

fractional change of a quantity

A term which may be expressed infinitesimally at time t by the differential $\frac{\mathrm{d}Q(t)}{Q(t)}$. For a finite time interval the quotient is

$$\frac{\Delta Q(t_1;\, t_2)}{Q(t_1)} = \frac{[Q(t_2) - Q(t_1)]}{Q(t_1)}$$

The quantities $Q(t_1)$ and $Q(t_2)$ are of the same kind and have the same type of component. Fractional change has dimension one. Examples are: mass fractional change, $\frac{\mathrm{d}m(t)}{m(t)}$; amount of substance fractional change, $\frac{\mathrm{d}n(t)}{n(t)}$.

Source:

PAC, 1992, *64*, 1569 *(Quantities and units for metabolic processes as a function of time (IUPAC Recommendations 1992))* on page 1571

fractional selectivity

in catalysis

The term selectivity (S) is used to describe the relative rates of two or more competing reactions on a catalyst. Such competition includes cases of different reactants undergoing simultaneous reactions or of a single reactant taking part in two or more reactions. For the latter case, S may be defined in two ways. The first of these defines a fractional selectivity, S_F, for each product by the equation

$$S_{\mathrm{F}} = \frac{\xi_i}{\sum \xi_i}$$

The second defines relative selectivities, S_{R}, for each pair of products by

$$S_{\mathrm{R}} = \frac{\xi_i}{\xi_j}$$

In each case, ξ_i and ξ_j are the rates of increase of the extent of reactions i and j respectively, i.e.

$$\xi_i = \frac{\mathrm{d}\xi_i}{\mathrm{d}t}$$

and

$$\xi_j = \frac{\mathrm{d}\xi_j}{\mathrm{d}t},$$

where ξ_i and ξ_j are the extents of reactions i and j respectively.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 81

fractionation

of analytes

Process of classification of an analyte or a group of analytes from a sample according to physical (*e.g.*, size, solubility) or chemical (*e.g.*, bonding, reactivity) properties.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1052

fractionation

of polymers

A process by means of which macromolecular species differing in some characteristic (chemical composition, relative molecular mass, branching, stereoregularity, etc.) are separated from each other.

Source:
Purple Book, p. 68

fragment ion

in mass spectrometry

An electrically charged dissociation product of an ionic fragmentation. Such an ion may dissociate further to form other electrically charged molecular or atomic moieties of successively lower formula weight.
See also: daughter ion

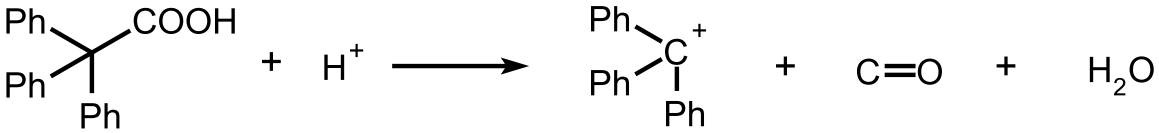
Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549
Orange Book, p. 205
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2190

fragmentation

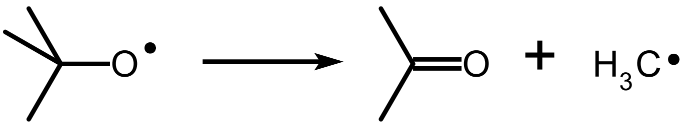
1. The heterolytic cleavage of a molecule according to the general reaction:

$$\mathrm{a{-}b{-}c{-}d{-}X} \longrightarrow (\mathrm{a{-}b})^{+} + \mathrm{c{=}d} + \mathrm{X}^{-}$$

where a-b is an electrofuge and X is a nucleofuge (which may emerge from the reaction in combined form), and the middle group affords the unsaturated fragment c=d. For example,

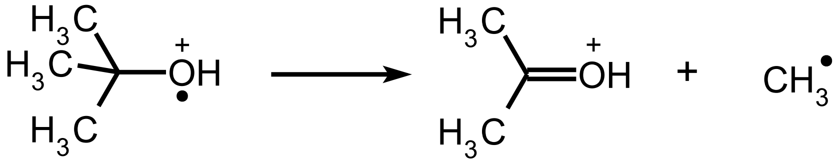


2. The breakdown of a radical into a diamagnetic molecule or ion and a smaller radical, e.g.



$$[\mathrm{ArBr}]^{\bullet-} \longrightarrow \mathrm{Ar} + \mathrm{Br}^{-} \quad \text{(solution)}$$

3. The breakdown of a radical ion in a mass spectrometer or in solution, forming an ion of lower molar mass and a radical, e.g.



See also: fragmentation reaction *in mass spectrometry*

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1116

fragmentation reaction

in mass spectrometry

A fragmentation reaction may be written:

$$\mathrm{M}_1^+ \rightarrow \mathrm{M}_2^+ + \mathrm{M}_3$$

The decomposition of a metastable ion of mass-to-charge ratio $\frac{m_1}{z_1}$ into an ion of mass-to-charge ratio $\frac{m_2}{z_2}$ after electric acceleration of the metastable ion and before magnetic deflection gives rise to a peak in the mass spectrum at an apparent mass, $\frac{{m_2}^2\,z_1}{m_1\,{z_2}^2}$. The symbol m^* should be used to indicate the apparent mass of the product ions giving rise to this peak. Traditionally, the peak itself has been called a metastable peak and this should preferably be expressed as metastable ion peak. It is nevertheless recommended that the former term should be retained. The word metastable should never be used as a noun. Its use as an adjective should be limited to such terms as metastable ion, where it is used correctly, and to the special case of metastable peak discussed above. It should never be used in such terms as metastable reaction, metastable decomposition, metastable studies, etc. It should be clear that the metastable ion is the ion that undergoes fragmentation; it is not detected. When a reaction is written with an asterisk above the arrow as shown:

$$\mathrm{M}_1^+ \overset{*}{\rightarrow} \mathrm{M}_2^+ + \mathrm{M}_3$$

this means that the reaction has been confirmed by the observation of a metastable peak. The textual description of such a process may be written as, for example, (m^*, $43 \rightarrow 28$, calcd. 18.2, obsd. 18.3) meaning 'for the fragmentation $\frac{m}{z}\ 43 \rightarrow \frac{m}{z}\ 28$ a metastable peak at $\frac{m}{z}$ 18.3 (calculated 18.2) has been observed'.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1557

frame-shift mutation

A point mutation involving either the deletion or insertion of a nucleotide in a gene. By the frame-shift mutation, the normal reading frame used when decoding the nucleotide triplets in the gene is altered to another reading frame.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 154

Franck–Condon principle

Also contains definitions of: Franck–Condon state, vertical transition

Classically, the Franck–Condon principle is the approximation that an electronic transition is most likely to occur without changes in the positions of the nuclei in the molecular entity and its environment. The resulting state is called a Franck–Condon state, and the transition involved, a vertical transition. The quantum mechanical formulation of this principle is that the intensity of a vibronic transition is proportional to the square of the overlap integral between the vibrational wavefunctions of the two states that are involved in the transition.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2243

franklin

esu unit of electric charge, $\mathrm{Fr} \approx 3.335\ 64 \times 10^{-10}\ \mathrm{C}$.

Source:
Green Book, 2nd ed., p. 114

free charge density on the interface

The physical charge density believed to occur on either side of the electrical double-layer.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 508

free electron laser

Source of coherent radiation in which the active medium is an electron beam moving at speeds close to the speed of light in the spatially periodic magnetic field produced by an array of magnets (the wiggler). The emitted wavelength, λ_{L}, is approximately given by

$$\frac{\lambda_{\omega}}{4\,E^2},$$

with λ_{ω} being the wiggler period and E the electron's energy in MeV.
See: laser

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2244

free energy

See: Gibbs energy (function)

Source:
Green Book, 2nd ed., p. 48
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 975
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2192

free radical

See: radical

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1116
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2190

free rotation (hindered rotation, restricted rotation)

In a stereochemical context the rotation about a bond is called 'free' when the rotational barrier is so low that different conformations are not perceptible as different chemical species on the time scale of the experiment. The inhibition of rotation of groups about a bond due to the presence of a sufficiently large rotational barrier to make the phenomenon observable on the time scale of the experiment is termed hindered rotation or restricted rotation.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2209

free-running laser

A term applied to a pulsed laser, meaning that the laser emission lasts as long as the pumping process is sufficient to sustain lasing conditions. Typical pulse durations are in the μs-ms range, depending on the pumping source. When the operation mode of a pulsed laser is not specified as mode-locked, Q-switched, or anything else, it must be considered as free-running.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2244

freely draining

An adjective referring to a chain macromolecule the segments of which produce such small frictional effects when moving in a medium that the hydrodynamic field in the vicinity of a given segment is not affected by the presence of other segments. Thus, the solvent can flow virtually undisturbed through the domain occupied by a freely draining macromolecule.

Source:
Purple Book, p. 61

freely jointed chain

in polymers

A hypothetical linear chain molecule consisting of infinitely thin rectilinear segments uniform in length; each segment can take all orientations in space with equal probability, independently of its neighbours. For models in which the segments are not all uniform in length, the name 'random-walk chain' has been used.

Source:
Purple Book, p. 50

freely rotating chain

in polymers

A hypothetical linear chain molecule, free from short-range and long-range interactions, consisting of infinitely thin rectilinear segments (bonds) of fixed length, jointed at fixed bond angles; the torsion angles of the bonds can assume all values with equal probability.

Source:
Purple Book, p. 50

freezing

The conversion of a liquid to a solid by lowering the temperature and/or the application of pressure.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 583

freezing out

in atmospheric chemistry

A term used in combustion for the analysis of incinerator flue gas components (largely the organic fraction) in which a series of traps at progressively lower temperatures is employed. In more general use, the term implies the removal of a condensable gas or liquid by condensation in a trap at low temperatures.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2190

frequency, f, ν

Reciprocal of the period.

Source:
Green Book, 2nd ed., p. 11

See also:
frequency in photochemistry
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 974
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2244

frequency, ν, ω

in photochemistry

The number of waveperiods per time interval. The linear frequency, ν, is the number of cycles per time interval. SI unit $\mathrm{Hz} = \mathrm{s}^{-1}$.
Note:
For the angular frequency the symbol ω ($= 2\,\pi\,\nu$) is used with $\mathrm{rad\ s}^{-1}$ as the SI unit.
See also: a more general definition of frequency

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 345

frequency distribution

If the range of observed measurement values is subdivided into a regular sequence of smaller intervals, this distribution is a plot of the frequency of occurrence of values falling into each interval.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2190

frequency doubling

See: harmonic frequency generation, non-linear optical effects

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2244

frequency-domain fluorometry

Technique that permits recovery of the parameters characterizing a fluorescence decay. Instead of using an exciting visible, UV, or infrared radiation pulse (see single-photon timing), the sample is excited by sinusoidally modulated radiation at high frequency. The fluoresence response is sinusoidally modulated at the same frequency as, but delayed in phase and partially demodulated with respect to the excitation.

Notes:

1. The modulation ratio is defined as the ratio is defined as the ratio of the modulation depth (AC/DC ratio) of the fluorescence and the modulation depth of the excitation. The phase shift and the modulation ratio characterize the harmonic response of the system. These parameters are measured as a function of the modulation frequency. No deconvolution is necessary because the data are directly analysed in the frequency domain.
2. Phase and modulation measurements can be done by using either a CW laser (or a xenon lamp) and an optical modulator (in general a Pockel cell) or the harmonic content of a pulsed laser.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 346

FRET

Acronym for Förster-resonance-energy transfer.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 346

friction factor, μ

Synonym: friction coefficient

Quotient of frictional force and normal force, for a sliding body. Formerly called frictional coefficient or coefficient of friction.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 974

frictional coefficient, f

in polymer chemistry

A tensor correlating the frictional force, $\boldsymbol{F}$, opposing the motion of a particle in a viscous fluid and the velocity $\boldsymbol{u}$ of this particle relative to the fluid. In the case of an isolated spherical particle in a viscous isotropic fluid, $\boldsymbol{f}$ is a constant and $\boldsymbol{F} = \boldsymbol{f}\,\boldsymbol{u}$.

Source:
Purple Book, p. 60

fringed-micelle model

in polymer crystals

A model of crystallinity in which the crystallized segments of a macromolecule belong predominantly to different crystals.

Source:
Purple Book, p. 84

front surface geometry

in luminescence

A system where excitation and observation are from the same face of the sample ($\alpha \angle 90\,^\circ$, $\beta \angle 180\,^\circ$ where α = angle of incidence of the exciting beam on the plane surface of the sample, and β = angle between the exciting direction and observation direction.)

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 244

frontal chromatography

A procedure in which the sample (liquid or gas) is fed continuously into the chromatographic bed. In frontal chromatography no additional mobile phase is used.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 824

frontier orbitals

Also contains definition of: LUMO

The *H*ighest-energy *O*ccupied *M*olecular *O*rbital (HOMO) (filled or partly filled) and *L*owest-energy *U*noccupied *M*olecular *O*rbital (LUMO) (completely or partly vacant) of a molecular entity. Examination of the mixing of frontier molecular orbitals of reacting molecular entities affords an approach to the interpretation of reaction behaviour; this constitutes a simplified perturbation molecular orbital theory of chemical behaviour.
See also: SOMO, subjacent orbital

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1116

fronting

in chromatography

Asymmetry of a peak such that, relative to the baseline, the front is less steep than the rear. In paper chromatography and thin-layer chromatography, it refers to the distortion of a spot showing a diffuse region in front of the spot in the direction of flow.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 837

Orange Book, p. 96

frost point hygrometer

Instrument in which the sample is passed over a cooled surface. The temperature at which frost forms on it is a function of the water content of the gas passing over the surface.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

froth flotation

The removal of particulate matter by foaming.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 609

Frumkin effect

Also contains definition of: 'true' rate constant

In an electrode reaction, when reactants or intermediates are adsorbed, the rate of reaction may no longer be related to the concentration by a simple law. The deviation may be due to either entropic or energetic effects or both. The situation best understood is that where a reactant is non-specifically adsorbed in the outer Helmholtz plane (inner boundary of the diffuse layer). The effect of such adsorption on electrode kinetics is usually termed the Frumkin effect. Rate constants, transfer coefficients etc. corrected for this effect are frequently called 'true' rate constants etc. It would be preferable to describe them as 'corrected for the Frumkin effect', but in any case, if such a correction is carried out, the basis on which it is made should be clearly described.

Source:
PAC, 1980, *52*, 233 *(Electrode reaction orders, transfer coefficients and rate constants. Amplification of definitions and recommendations for publication of parameters)* on page 239

fucolipid

See: glycolipids

Source:
White Book, p. 184

fuel cycle (nuclear)

The sequence of steps, such as utilization, reprocessing, and refabrication, through which nuclear fuel may pass.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

fuel element (nuclear)

The smallest structurally discrete part of a reactor which has fuel as its principal constituent.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

fuel reprocessing (nuclear)

The processing of nuclear fuel, after its use in a reactor, to remove fission products and recover fissile and fertile material.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

fugacity, f, $\tilde{p}$

Of a substance **B**, f_{B} or $\widetilde{p_{\mathrm{B}}}$, in a gaseous mixture is defined by $f_{\mathrm{B}} = \lambda_{\mathrm{B}} \lim\limits_{p \to 0} \frac{p_{\mathrm{B}}}{\lambda_{\mathrm{B}}}$, where p_{B} is the partial pressure of B and λ_{B} its absolute activity.

Source:
Green Book, 2nd ed., p. 50

See also:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 539
PAC, 1984, *56*, 567 *(Physicochemical quantities and units in clinical chemistry with special emphasis on activities and activity coefficients (Recommendations 1983))* on page 571

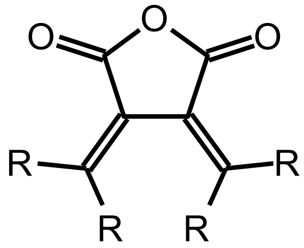
fugacity coefficient, ϕ

Ratio of fugacity to the partial pressure of a gaseous constituent.

Source:
Green Book, 2nd ed., p. 50
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 539

fulgides

Dialkylidenesuccinic anhydrides (generally photochromic).



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

full energy peak

Synonym: total absorption peak

Of a spectrum of radiation, the part of the spectral response curve corresponding to the total absorption in a detecting material of the energy of the detected radiation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

fullerenes

Compounds composed solely of an even number of carbon atoms, which form a cage-like fused-ring polycyclic system with twelve five-membered rings and the rest six-membered rings. The archetypal example is [60]fullerene, where the atoms and bonds delineate a truncated icosahedron. The term has been broadened to include any closed cage structure consisting entirely of three-coordinate carbon atoms.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

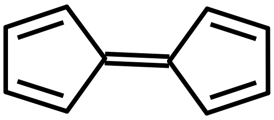
fulminates

1. Compounds having the structure RON=C:. So called because fulminic acid (actually $HC{\equiv}N^{+}$–O^{-} formonitrile oxide) was previously considered to be HON=C:.
2. Salts of fulminic acid, e.g. $Na^{+}[–C{\equiv}N^{+}O^{-}]$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

fulvalenes

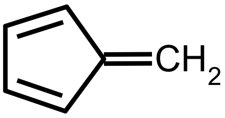
The hydrocarbon fulvalene and its derivatives formed by substitution (and by extension, analogues formed by replacement of one or more carbon atoms of the fulvalene skeleton by a heteroatom).



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

fulvenes

The hydrocarbon fulvene and its derivatives formed by substitution (and by extension, analogues formed by replacement of one or more carbon atoms of the fulvene skeleton by a heteroatom).



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

fume

in atmospheric chemistry

Fine solid particles (aerosol), predominantly less than 1 μm in diameter, which result from the condensation of vapour from some types of chemical reaction. Usually this is formed from the gaseous state generally after volatilization from melted substances and often accompanied by chemical reactions such as oxidation.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2190

fumes

In popular usage, a term often taken to mean airborne effluents, unpleasant and malodorous, which might arise from chemical processes.
See also: smoke

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

fumigation

in atmospheric chemistry

An atmospheric phenomenon in which pollution, retained by an inversion layer near its level of emission, is brought rapidly to ground level as the inversion breaks up. This term also applies to the exposure of material (e.g. grain) to chemicals to kill insects, etc.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

functional class name

A name that expresses the characteristic group as a class term written as a separate word following the name of a parent structure or a name derived from a parent structure. In the latter case, when the derived name is that for a substituent group (formerly called a 'radical'), the method has been called 'radicofunctional nomenclature'.

Source:
Blue Book (Guide), p. 14

functional group

Organic compounds are thought of as consisting of a relatively unreactive backbone, for example a chain of sp^3 hybridized carbon atoms, and one or several functional groups. The functional group is an atom, or a group of atoms that has similar chemical properties whenever it occurs in different compounds. It defines the characteristic physical and chemical properties of families of organic compounds.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1116

functional parent

A structure the name of which implies the presence of one or more characteristic groups and which has one or more hydrogen atoms attached to at least one of its skeletal atoms or one of its characteristic groups, or in which at least one of its characteristic groups can form at least one kind of functional modification.
Note:
A parent hydride bearing a characteristic group denoted by a suffix, for example, cyclohexanol, is not considered to be a functional parent, but may be described as a 'functionalized parent hydride'.

Source:
Blue Book (Guide), p. 13

functional polymer

1. Polymer that bears specified chemical groups or
2. polymer that has specified physical, chemical, biological, pharmacological, or other uses which depend on specific chemical groups.

Note:
Examples of functions of functional polymers under definition 2. are catalytic activity, selective binding of particular species, capture and transport of electric charge carriers or energy, conversion of light to charge carriers and *vice versa*, and transport of drugs to a particular organ in which the drug is released.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 899

functionality, f

of a monomer

Number of covalent bonds that a monomer molecule or monomeric unit in a macromolecule or oligomer molecule can form with other reactants.

Notes:
1. There are no monofunctional monomers.
2. If $f = 2$, a linear chain macromolecule or a macrocycle can be formed.
3. If $f > 2$, a branch point can be formed leading to a branched macromolecule, a network or a micronetwork.
4. Ethene and ethylene glycol are examples of difunctional monomers, glycerol is an example of a trifunctional monomer, and divinylbenzene and pentaerythritol are examples of tetrafunctional monomers.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1805

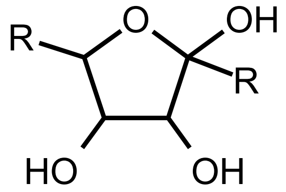
furanocoumarins

An alternative name for furocoumarins.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

furanoses

Cyclic hemiacetal forms of monosaccharides in which the ring is five-membered (i.e. a tetrahydrofuran skeleton).



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1336

furnace black

A type of carbon that is produced industrially in a furnace by incomplete combustion in an adjustable and controllable process that yields a wide variety of properties within the product.
Note:
The most widely employed industrial process for carbon black production is the furnace process.
See also: gas black

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 490

furnace pyrolysis

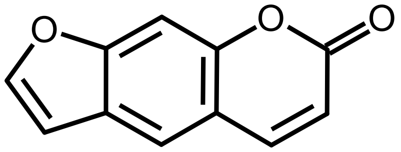
in spectrochemical analysis

A flowing stream of gas (hydrogen, oxygen, nitrogen, chlorine, etc.) required to produce volatile species of the elements being determined, is passed over the test sample in a heated furnace. The analytes leave the furnace in the gas stream, or are entrained by a carrier gas. The analytes in the gas stream may be collected in an absorbing solution, on a carbon or other filter or by condensation on a cool surface. In the case of mercury this can also be done by amalgamation with a noble metal. The analytes may then be swept and released from the trap, by heating, into a sampling source for analysis.

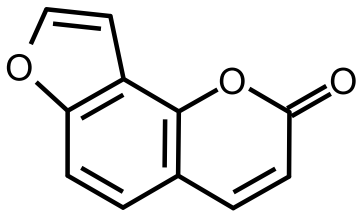
Source:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1470

furocoumarins

Derivatives (mostly of natural origin) of the linear furocoumarin skeleton, psoralen, or its angular isomer, angelicin, variously substituted with hydroxy, methoxy, alkyl, or hydroxymethyl groups, among others.



psoralen



angelicin

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

fusion

in biotechnology

The amalgamation of two distinct cells or macromolecules into a single integrated unit.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 154

fusion name

A composite name for a polycyclic parent structure having the maximum number of non-cumulative double bonds and at least one *ortho* fusion. Name formation involves the dissection of the structure into contiguous components having recognized trivial or semisystematic names, one of which is selected as the 'base component'. Attachment of the other components is described by prefixes.

Source:
Blue Book (Guide), p. 14

FWHM (Full Width at Half Maximum)

See: half-width *of a band*, line width

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2244
Green Book, 2nd ed., p. 31

See also:
Orange Book, p. 226

γ-cascade

Two or more different gamma rays emitted successively from one nucleus when it passes through one or more energy levels.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

γ-quantum

A photon of γ-radiation

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

γ-radiation

Electromagnetic radiation emitted in the process of nuclear transformation or particle annihilation

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

γ-ray spectrometer

A measuring assembly for determining the energy spectrum of γ-rays.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

G value

in nuclear chemistry

The number of specified chemical events in an irradiated substance produced per $100\ \mathrm{eV}$ of energy absorbed from ionizing radiation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1544

gain, G

of a photomultiplier

The gain of a photomultiplier is given by the equation $G = k\,\sigma^n$, where k is the efficiency of collection of photoelectrons on the first dynode, σ is the secondary emission ratio, i.e. the number of secondary electrons emitted for each electron incident on the dynode and n is the number of dynodes.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1753

Galvani potential difference

An electric potential difference between points in the bulk of two phases. It is measurable only when the two phases have identical composition (e.g. two copper wires). It is the difference of inner electric potentials in two phases. Symbol: $\Delta_{\alpha}^{\beta}\phi$.

Source:
Green Book, 2nd ed., p. 59

galvanic corrosion

See: contact corrosion

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 22

gas analysis installation

in atmospheric chemistry

An assembly for the purpose of determining one or more components in a gaseous mixture. It generally comprises the following elements: sample probe, region of primary treatment of the gases, region of secondary treatment of gases, points for venting to the atmosphere and for calibration sample injection, transfer line and the analytical unit.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

gas black (carbon black, channel black, furnace black)

Finely divided carbon (graphite) produced by incomplete combustion or thermal decomposition of natural gas.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

gas chromatography (GC)

A separation technique in which the mobile phase is a gas. Gas chromatography is always carried out in a column.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 825
Orange Book, p. 93
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

gas constant

Fundamental physical constant, $R = 8.314\,472\ (15)\ \mathrm{J\ K^{-1}\ mol^{-1}}$.

Source:
CODATA 2006
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 974

gas laser

A laser in which the active medium is a gas containing a laser active species. It is typically composed of a plasma discharge tube containing a gas that can be excited with an electric discharge.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1919

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2244

gas sensing electrode

A sensor composed of an indicator and a reference electrode in contact with a thin film of solution which is separated from the bulk of the sample solution by a gas-permeable membrane or an air gap. This intermediate solution interacts with the gaseous species (penetrated through the membrane or an air gap) in such a way as to produce a change in a measured constituent (e.g. the H^+ activity) of the intermediate solution. This change is then sensed by the ion-selective electrode and is related to the partial pressure of the gaseous species in the sample. [Note: In electrochemical literature the term gas electrode is used for the classical, redox-equilibrium-based gas electrodes as well, such as the hydrogen or the chlorine gas electrodes (Pt (s)|H_2 (g) | H^+ (aq) or Pt (s) |Cl_2 (g) | Cl^- (aq)]. These electrodes respond both to the partial pressure of the gas (H_2 or Cl_2) and to the ionic activities (H^+

or Cl^{-}). The Clark oxygen electrode fits under this classification although, in contrast to other gas sensors, it is an amperometric and not a potentiometric device.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2534

gas-filled phototube

Similar in construction to a vacuum phototube except that it is filled with a noble gas (usually Ar) at a pressure of about $10\ \mathrm{Pa}$. Photoelectrons accelerated by the anode electric potential ionize gas atoms. The additional electrons provide a substantial intrinsic gain.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1753

gas-filled X-ray detector

A cylindrical cathode with a window, an axial wire anode and an ionizable gas. The gas may be continuously replenished giving a flow-through detector or the detector may be sealed. Following an original ionizing event, electron multiplication occurs through a process of gas amplification in the high electric field surrounding the anode wire. The gain of this process is defined as the number of electrons collected on the anode wire for each primary electron produced. For X-rays having energies higher than the excitation potential of the detector gas, the spectral responsivity function has a second peak in addition to the main peak that is called the escape peak. The escape peak has a mean pulse height proportional to the difference between the photon energy of the incident X-rays and of the spectral characteristic line of the detector gas. A quenching gas, a molecular gas, is added to the detector gas in order to neutralize the detector gas ions and to absorb secondary electrons as well as UV radiation resulting from neutralization of detector gas ions. According to the potential applied to the anode, the detector can work as an ionization chamber, proportional counter, or Geiger counter.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1753

gas-liquid chromatography

Comprises all gas-chromatographic methods in which the stationary phase is a liquid dispersed on a solid support. Separation is achieved by partition of the components of a sample between the phases.

Source:
Orange Book, p. 93

gas-phase acidity

The negative of the Gibbs energy ($\Delta G_{\mathrm{r}}{}^{\circ}$) change for the reaction:

$$\mathrm{A{-}H} \longrightarrow \mathrm{A^{-}} + \mathrm{H^{+}}$$

in the gas phase.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1116

gas-phase basicity

The negative of the Gibbs energy ($\Delta G_{\mathrm{r}}{}^{\circ}$) change associated with the reaction:

$$\mathrm{B} + \mathrm{H^{+}} \longrightarrow \mathrm{\overset{+}{B}{-}H}$$

in the gas phase. Also called absolute or intrinsic basicity.
See also: proton affinity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1116

gas-phase-grown carbon fibres

Carbon fibres grown in an atmosphere of hydrocarbons with the aid of fine particulate solid catalysts such as iron or other transition metals and consisting of graphitizable carbon.
Note:
Gas-phase-grown carbon fibres transform during graphitization heat treatment into graphite fibres. These show a very high degree of preferred orientation and are particularly suitable for intercalation treatments. The term 'vapour-grown carbon fibres' alternatively used in the literature is acceptable. The use of the term 'CVD fibres' is not recommended as an alternative for gas-phase-grown carbon fibres since the term 'CVD fibres' also describes fibres grown by a chemical vapour deposition (CVD) process on substrate fibres.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 490

gas-solid chromatography

Comprises all gas chromatographic methods in which the stationary phase is an active solid (e.g. charcoal, molecular sieves). Separation is achieved by adsorption of the components of a sample. In gas chromatography the distinction between gas-liquid and gas-solid may be obscure because liquids are used to modify solid stationary phases, and because the solid supports for liquid stationary phases affect the chromatographic process. For classification by the phases used, the term relating to the predominant effect should be chosen.

Source:
Orange Book, p. 93

gaseous diffusion separator

in atmospheric chemistry

Instrumentation to separate a gas mixture into its components by means of differences in the diffusion rates of the component molecules. This method has been used in separation of various isotopes of uranium (by means of UF_6) and hydrogen (H_2O, HDO, D_2O, HTO, etc.)

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2192

gated photochromism

Special form of photochromism in which one or both forms of a photochromic system are transformed reversibly, either chemically or electrochemically, into a non-photochromic form.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 347

gated photodetector

Where photodetectors are switched on (or off) usually in a repetitive manner employing electronic switches, they are described as gated.

Source:
Orange Book, p. 193

gauche

Synonymous with a synclinal alignment of groups attached to adjacent atoms.
See: torsion angle

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2209
Blue Book, p. 484

gauche conformation

in polymers

See: cis conformation *in polymers*

Source:
Purple Book, p. 41

gauche effect

1. The stabilization of the gauche (synclinal) conformation in a two carbon unit bonded vicinally to electronegative elements e.g. 1,2-difluoroethane.
2. The destabilization of the gauche (synclinal) conformation in a two carbon unit bonded vicinally to large, soft and polarizable elements such as sulfur and bromine.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2209

gauss

emu unit of magnetic flux density, $\mathrm{G} = 10^{-4}\,\mathrm{T}$.

Source:
Green Book, 2nd ed., p. 115

Gaussian band shape

A band shape described by the Gaussian function:

$$F(\nu - \nu_0) = \frac{a}{\sqrt{\pi}}\, \mathrm{e}^{-a^2 (\nu-\nu_0)^2}$$

In this equation, a^{-1} is proportional to the width of the band, and ν_0 is the frequency of the band maximum.
See also: Lorentzian band shape

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2244

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2192

Geiger counter

A gas-filled X-ray detector in which gas amplification reaches saturation and proportionality no longer exists. The output signal does not depend on the incident energy. The time taken for the counter to recover from the saturation is called dead time.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1754

Geiger–Muller counter tube

A counter tube operated under such conditions that the magnitude of each pulse is independent of the amount of energy deposited in it.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

gel

Non-fluid colloidal network or polymer network that is expanded throughout its whole volume by a fluid.
Notes:

1. A gel has a finite, usually rather small, yield stress.
2. A gel can contain:
   1. a covalent polymer network, e.g., a network formed by crosslinking polymer chains or by non-linear polymerization;
   2. a polymer network formed through the physical aggregation of polymer chains, caused by hydrogen bonds, crystallization, helix formation, complexation, *etc*, that results in regions of local order acting as the network junction points. The resulting swollen network may be termed a thermoreversible gel if the regions of local order are thermally reversible;
   3. a polymer network formed through glassy junction points, e.g., one based on block copolymers. If the junction points are thermally reversible glassy domains, the resulting swollen network may also be termed a thermoreversible gel;
   4. lamellar structures including mesophases, e.g., soap gels, phospholipids and clays;
   5. particulate disordered structures, e.g., a flocculent precipitate usually consisting of particles with large geometrical anisotropy, such as in V_2O_5 gels and globular or fibrillar protein gels.
3. Corrected from previous definition where the definition is *via* the property identified in Note 1 (above) rather than of the structural characteristics that describe a gel.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1806

gel aging

Time-dependent changes in the chemical or the physical structure and the properties of a gel.
Note:
The aging of a gel can involve polymerization, crystallization, aggregation, syneresis, phase changes, formation of branch points and junction points as well as scission and chemical changes to constitutional units of network chains.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1823

gel fraction

Mass fraction of the network material resulting from a network-forming polymerization or crosslinking process.
Note:
The gel fraction comprises a single molecule spanning the entire volume of the material sample.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1811

gel point

Also contains definition of: gelation point

Point of incipient network formation in a process forming a chemical or physical polymer network.
Notes:
1. In both network-forming polymerization and the crosslinking of polymer chains, the gel point is expressed as an extent of chemical reaction (*c.f.,* gel time).
2. At the gel point a solid (network) material spanning the entire system is formed.
   See also: gel fraction
3. The gel point is often detected using rheological methods. Different methods can give different gel points because viscosity is tending to infinity at the gel point and a unique value cannot be measured directly.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1809

gel time

Also contains definition of: gelation time

Time interval from the start of a network-forming process to the gel point.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1809

gelation

Process of passing through the gel point to form a gel or network.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1823

gelation temperature

Also contains definition of: gel temperature

Temperature threshold for the formation of a thermoreversible gel.
Notes:

1. A thermoreversible gel is usually formed by cooling a polymer solution. In these cases, the gel temperature is a maximum temperature at which the presence of network is observed.
2. Since gel temperatures depend on the method of determination, this should always be indicated.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1809

geminate ion pair

Ion pair formed from a precursor that constitutes a single kinetic entity, i.e., by electron transfer or ion transfer in an encounter complex (cf. collision complex) or by ionic dissociation of a single molecular entity.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 347

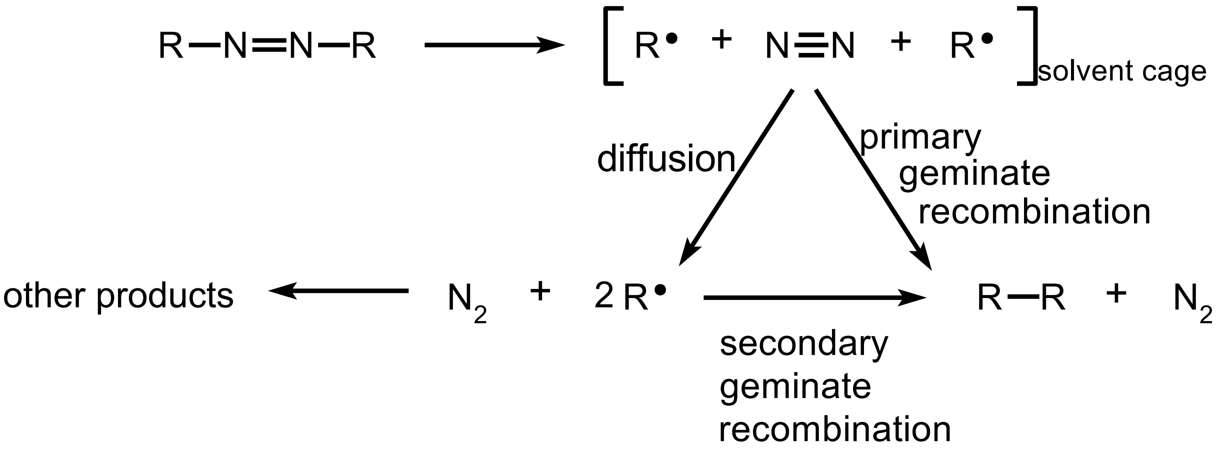
geminate pair

Pair of molecular entities in close proximity in solution within a solvent cage and resulting from reaction (e.g. bond scission, electron transfer, group transfer) of a precursor that constitutes a single kinetic entity.
See also: ion pair, radical pair

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1117

geminate recombination

This expression refers to the reaction, with each other, of two transient species produced from a common precursor in solution. If reaction occurs before any separation by diffusion has occurred, this is termed primary geminate recombination. If the mutually reactive entities have been separated, and come together by diffusion, this is termed secondary geminate recombination. This is illustrated in the reaction diagram below:



See also: cage

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 166
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1117

gene amplification

An increase in the number of copies of a specific gene in an organism. This can lead to the production of a corresponding protein at elevated levels.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 154

gene (cistron)

Structurally, a basic unit of hereditary material; an ordered sequence of nucleotide bases that encodes one polypeptide chain (via mRNA). The gene includes, however, regions preceding and following the coding region (leader and trailer) as well as (in eukaryotes) intervening sequences (introns) between individual coding segments (exons). Functionally, the gene is defined by the *cis-trans* test that determines whether independent mutations of the same phenotype occur within a single gene or in several genes involved in the same function.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 154

gene library

A collection of cloned DNA fragments from a variety of species.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 155

gene manipulation

The use of *in vitro* techniques to produce DNA molecules containing novel combinations of genes or altered sequences, and the insertion of these into vectors that can be used for their incorporation into host organisms or cells in which they are capable of continued propagation of the modified genes.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 155

general acid catalysis

The catalysis of a chemical reaction by a series of Brønsted acids (which may include the solvated hydrogen ion) so that the rate of the catalysed part of the reaction is given by $\sum k_{\mathrm{HA}}\,[\mathrm{HA}]$ multiplied by some function of substrate concentrations. (The acids HA are unchanged by the overall reaction.) General catalysis by acids can be experimentally distinguished from specific catalysis by hydrogen cations (hydrons) by observation of the rate of reaction as a function of buffer concentration.
See also: catalytic coefficient, intramolecular catalysis, pseudo-catalysis

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1117

general acid–base catalysis

Catalysis by acids or bases in solution is said to be general when it is possible to detect catalysis brought about by species other than the ions formed from the solvent itself (e.g. when water is the solvent, by species other than H^+ and OH^- ions).
See: general acid catalysis, general base catalysis

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 150

general base catalysis

The catalysis of a chemical reaction by a series of Brønsted bases (which may include the lyate ion) so that the rate of the catalysed part of the reaction is given by $\sum k_{\mathrm{B}}\,[\,\mathrm{B}\,]$ multiplied by some function of substrate concentration.
See also: general acid catalysis

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1117

general force field

Acronym: gff

A force field expressed in terms of $3\,N-6$ basis coordinates:

$$V=\frac{1}{2}\sum f_{ij}S_iS_j$$

$$V=\frac{1}{2}\sum F_{ij}S_iS_j$$

where f_{ij} (or F_{ij}) are force constants and the basis coordinates S (or sometimes s) may be internal symmetry coordinates, local symmetry coordinates or any others suitable to the problem, but the number of the coordinates has to be reduced to $3\,N-6$ ($3\,N-5$ for linear molecules), N being the number of atoms in the molecule.

Source:
PAC, 1978, *50*, 1707 *(Definition and symbolism of molecular force constants)* on page 1709

generalized transition-state theory

Any form of transition-state theory (TST), such as microcanonical variational TST, canonical variational TST, and improved canonical variational TST, in which the transition state is not necessarily located at the saddle point, is referred to as generalized transition-state theory.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 166

generally labelled tracer

A tracer in which the position of the label is not defined.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

generation time, t_G

in biotechnology

The average time required by a cell for the completion of one cell cycle.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 155

genetic algorithm

A genetic algorithm is a optimization algorithm based on the mechanisms of Darwinian evolution which uses random mutation, crossover and selection procedures to breed better models or solutions from an originally random starting population or sample.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1144

genetic code

The set of rules which governs the relationship between the linear order of the nucleotides in an mRNA molecule and the sequence of the amino acids in the protein which it encodes. The genetic code is a triplet code, nearly universal. It is not overlapping: a mutation which alters only a single nucleotide in a gene can change only one amino acid in the encoded protein. It is degenerate: it assigns each of the 20 amino acids to one or more of 61 of the 64 possible nucleotide triplets (cf. codon) that can be constructed from four nucleotides. The remaining three triplets are used to signal the termination of a genetic message.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 155

genome

The complete set of chromosomal and extrachromosomal genes of an organism, a cell, an organelle or a virus; the complete DNA component of an organism.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 155

genomics

1. Science of using DNA- and RNA-based technologies to demonstrate alterations in gene expression.
2. (*in toxicology*) Method providing information on the consequences for gene expression of interactions of the organism with environmental stress, xenobiotics, *etc*..

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1053

genotype

The genetic constitution of an organism as revealed by genetic or molecular analysis, i.e. the complete set of genes, both dominant and recessive, possessed by a particular cell or organism.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 155

geometric attenuation

The reduction of a radiation quantity due to the effect only of the distance between the point of interest and the source, excluding the effect of any matter present.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

geometric isomerism [obsolete]

Obsolete synonym for cis-trans isomerism. (Usage strongly discouraged).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2209

geometric (logarithmic) mean, $\bar{x}_\mathrm{g}$

The *n*th root of the product of the absolute values of the observations, taken with the proper sign. It can be calculated with the formula:

$$\bar{x}_\mathrm{g} = (\Pi \ | x_i |)^{\frac{1}{n}}$$

The Π product is taken from $i = 1$ to n.
Note:
This quantity is often calculated directly from experimental measurements (e.g. determination of concentrations by electrode potential measurements, or pH), although its significance may not always have been recognized. The problem is that the average value of a variable (such as pH) that is a function of concentration is not the same as the value of the function at the average concentration. In the case of electrode potentials, the average potential is equivalent to the geometric mean concentration. The correct procedure is to transform to units of concentration before averaging. There is one notable case where the geometric mean is appropriate, namely, when the analyte itself is distributed in a log-normal fashion, as in certain environmental and geological samples.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 602

geometrical equivalence

in polymers

The symmetry correspondence among units belonging to the same chain. The symmetry elements always bear a special relationship to the chain axis.
See also: line repetition groups

Source:
Purple Book, p. 77

geometry (counting)

in radioanalytical chemistry

A term used colloquially to signify the arrangement in space of the various components in an experiment, particularly the source and the detector in radiation measurements.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

geometry factor

in radioanalytical chemistry

The average solid angle in steradians at source subtended by the aperture or sensitive volume of the detector, divided by 4π.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

germylenes [obsolete]

See: germylidenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

germylidenes

Carbene analogues having the structure R_2Ge:. The older synonym germylenes is no longer recommended.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

Gibbs adsorption

The surface excess amount or Gibbs adsorption of component i, n_i^σ, which may be positive or negative, is defined as the excess of the amount of this component actually present in the system over that present in a reference system of the same volume as the real system and in which the bulk concentrations in the two phases remain uniform up to the Gibbs dividing surface. That is

$$n_i^\sigma = n_i - V^\alpha c_i^\alpha - V^\beta c_i^\beta$$

where n_i is the total amount of the component i in the system, c_i^α and c_i^β are the concentrations in the two bulk phases α and β, and V^α and V^β are the volumes of the two phases defined by the Gibbs surface.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 588

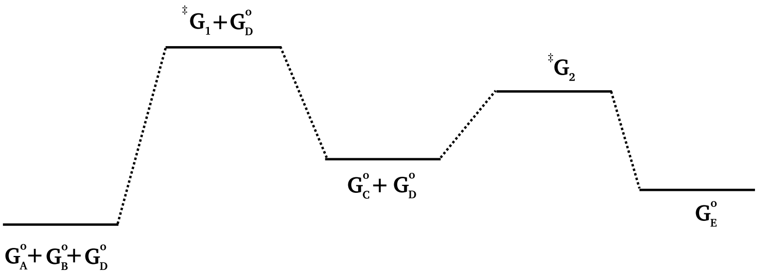
Gibbs energy diagram

A diagram showing the relative standard Gibbs energies of reactants, transition states, reaction intermediates and products, in the same sequence as they occur in a chemical reaction. These points are often connected by a smooth curve (a 'Gibbs energy profile', commonly still referred to as a 'free energy profile') but experimental observation can provide information on relative standard Gibbs energies only at the maxima and minima and not at the configurations between them. The abscissa expresses the sequence of reactants, products, reaction intermediates and transition states and is usually undefined or only vaguely defined by the reaction coordinate (extent of bond breaking or bond making). In some adaptations the abscissas are however explicitly defined as bond orders, Brønsted exponents, etc. Contrary to statements in many text books, the highest point on a Gibbs energy diagram does not necessarily correspond to the transition state of the rate-limiting step. For example, in a stepwise reaction consisting of two reaction steps:

$$1)\quad \mathrm{A} + \mathrm{B} \rightleftarrows \mathrm{C}$$

$$2)\quad \mathrm{C} + \mathrm{D} \longrightarrow \mathrm{E}$$

one of the transition states of the two reaction steps must (in general) have a higher standard Gibbs energy than the other, whatever the concentration of D in the system. However, the value of that concentration will determine which of the reaction steps is rate-limiting. If the particular concentrations of interest, which may vary, are chosen as the standard state, then the rate-limiting step is the one of highest Gibbs energy.



See also: potential energy profile, potential energy (reaction) surface

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1117
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 167

Gibbs energy (function), G

Enthalpy minus the product of thermodynamic temperature and entropy. It was formerly called free energy or free enthalpy.

Source:
Green Book, 2nd ed., p. 48
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 975
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2192

Gibbs energy of activation (standard free energy of activation), $\Delta^{\ddagger}G^{o}$

The standard Gibbs energy difference between the transition state of a reaction (either an elementary reaction or a stepwise reaction) and the ground state of the reactants. It is calculated from the experimental rate constant k *via* the conventional form of the absolute rate equation:

$$\Delta^{\ddagger}G = R\,T\left[\ln\left(\frac{k_{\mathrm{B}}}{h}\right) - \ln\left(\frac{k}{T}\right)\right]$$

where k_{B} is the Boltzmann constant and h the Planck constant ($\frac{k_{\mathrm{B}}}{h} = 2.083\ 58 \times 10^{10}\ \mathrm{K}^{-1}\ \mathrm{s}^{-1}$). The values of the rate constants, and hence Gibbs energies of activation, depend upon the choice of concentration units (or of the thermodynamic standard state).
See also: enthalpy of activation, entropy of activation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1118

PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 166

Gibbs energy of photoinduced electron transfer

For photoinduced electron transfer between an acceptor (A) and a donor (D) (either one of them may be the electronically excited molecular entity) of any charge type, $z(\mathrm{A})$ and $z(\mathrm{D})$, the change in standard Gibbs energy can be approximated as (the notation is for the case of neutral species D and A)

$$\Delta_{\mathrm{ET}}G^{\mathrm{o}} = N_{\mathrm{A}}\,\{e\,[E^{\mathrm{o}}(\mathrm{D}^{+\bullet}/\,\mathrm{D}) - E^{\mathrm{o}}(\mathrm{A}\,/\,\mathrm{A}^{-\bullet})] + w(\mathrm{D}^{+\bullet}\mathrm{A}^{-\bullet}) - w(\mathrm{DA})\} - \Delta E_{0,0}$$

where $e = 1.602\ 176\ 487 \times 10^{-19}\ \mathrm{C}$ is the elementary charge, $N_{\mathrm{A}} = 6.022\ 141\ 79 \times 10^{23}\ \mathrm{mol}^{-1}$ is the Avogadro constant, $E^{\mathrm{o}}(\mathrm{D}^{+\bullet}/\,\mathrm{D})/\mathrm{V}$ is the standard electrode potential of the donor cation radical resulting from the electron transfer, $E^{\mathrm{o}}(\mathrm{A}\,/\,\mathrm{A}^{-\bullet})/\mathrm{V}$ is the standard electrode potential of the acceptor (both relative to the same reference electrode) and $\Delta E_{0,0}/\mathrm{J\ mol}^{-1}$ is the vibrational zero electronic energy of the excited partner (provided that a vibrationally equilibrated excited state at energy $E_{0,0}$ takes part in the reaction), all data referring to the same solvent.

$w(\mathrm{D}^{+\bullet}\mathrm{A}^{-\bullet})$ and $w(\mathrm{DA})$ are the electrostatic work terms that account for the effect of Coulombic attraction in the products and reactants, respectively

$$w(\mathrm{D}^{+\bullet}\mathrm{A}^{-\bullet})/\mathrm{J} = \frac{z(\mathrm{D}^{+\bullet})\,z(\mathrm{A}^{-\bullet})\,e^2}{4\,\pi\,\varepsilon_0\,\varepsilon_{\mathrm{r}}\,a}$$

$$w(\mathrm{DA})/\mathrm{J} = \frac{z(\mathrm{D})\,z(\mathrm{A})\,e^2}{4\,\pi\,\varepsilon_0\,\varepsilon_{\mathrm{r}}\,a}$$

where a is the distance of the charged species after electron transfer, ε_{r} is the relative medium static permittivity (formerly called dielectric constant), $\varepsilon_0 \approx 8.854 \times 10^{-12}\ \mathrm{C}^2\ \mathrm{J}^{-1}\ \mathrm{m}^{-1}$ is the electric constant (vacuum permittivity), and $z(\mathrm{X})$ the charge of the species X.

In SI units the factor $\frac{e^2}{4\,\pi\,\varepsilon_0} = 2.307 \times 10^{-28}\ \mathrm{J\ m}$. For the case of neutral species A and D, $z(\mathrm{D}) = z(\mathrm{A}) = 0$.

Notes:

1. Several approximations are in use for the calculation of the term $w(\mathrm{D}^{+\bullet}\mathrm{A}^{-\bullet})$, depending on the nature of the species formed such as contact or solvent-separated radical ion pairs or extended and/or linked D and A molecular entities. In the latter case, the stabilization of a dipole μ in a cavity of radius ρ could be an appropriate model and

$$w(\mathrm{D}^{+\bullet}\mathrm{A}^{-\bullet}) = \frac{N_{\mathrm{A}}\,\mu^2}{4\,\pi\,\varepsilon_0\,\rho^3}\,\frac{\varepsilon_{\mathrm{r}} - 1}{2\,\varepsilon_{\mathrm{r}} + 1}$$

2. In the above definitions, the IUPAC recommendations for the sign and symbols of standard potentials are used. Although not complying with the IUPAC-recommended nomenclature for the standard electrode potentials, traditionally the equation has been written as:

$$\Delta_{\mathrm{ET}}G^{\mathrm{o}} = N_{\mathrm{A}} \left\{ e\,(E^{\mathrm{o}}_{\mathrm{ox}} - E^{\mathrm{o}}_{\mathrm{red}}) + \frac{[z(\mathrm{A}) - z(\mathrm{D}) - 1]\, e^2}{4\,\pi\,\varepsilon_0\,\varepsilon_{\mathrm{r}}\, a} \right\} - \Delta E_{0,0}$$

with $E^{\mathrm{o}}_{\mathrm{ox}}$ the standard electrode potential at which the oxidation occurs, and $E^{\mathrm{o}}_{\mathrm{red}}$ the standard electrode potential at which the reduction occurs. This form of the first term within the brackets is misleading and not recommended.

3. The standard emfs of oxidation and reduction are often called, respectively, 'oxidation' and 'reduction potential'. These terms are intrinsically confusing and should be avoided altogether, because they conflate the chemical concept of reaction with the physical concept of electrical potential.
4. The equation used for the calculation of the Gibbs energy of photoinduced electron-transfer processes should not be called the *Rehm-Weller equation*.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 348

Gibbs energy of repulsion

Indicated by G_{r} or G_{el} if the repulsion is due to electric effects (g_{r} or g_{el} is taken for unit area of each of two flat and parallel surfaces). G_{r} (or G_{el}) is defined as

$$G_{\mathrm{r}}\ (\text{ or } G_{\mathrm{el}}) = \left[\int_{\text{final distance}}^{\infty} \text{Force d(distance)} \right]_{T,p}$$

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 615

Gibbs energy profile

See: Gibbs energy diagram, transition-state theory

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1117
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 167
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 190

Gibbs film elasticity

Pertains to a film element of a soap film changing in area at constant mass and is the differential change of its surface tension with relative change in area A,

$$E = A \left(\frac{\partial \sigma}{\partial A}\right)_{T,p,n_i}$$

where T is the thermodynamic temperature, p is the pressure, and n_i is the amount of substance of the species i.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 615

Gibbs surface

Synonym: Gibbs dividing surface

A geometrical surface chosen parallel to the interface and used to define the volumes of the bulk phases in the calculation of the extent of adsorption, and of other surface excess properties. Also referred to as Gibbs dividing surface.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 588

giga

SI prefix for 10^9 (symbol: G).

Source:
Green Book, 2nd ed., p. 74

glass electrode error

Deviation of a glass electrode from the hydrogen-ion response function. An example often encountered is the error due to sodium ions at alkaline pH values, which by convention is regarded as positive.

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 540

glass laser

A solid state laser in which the active medium is a glass host that supports the active species. The neodymium-doped phosphate glass laser is one example.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1920

glass transition

A second-order transition in which a supercooled melt yields, on cooling, a glassy structure. Below the glass-transition temperature the physical properties vary in a manner similar to those of the crystalline phase. Example: Lithium disilicate crystals melt at $1305\ \mathrm{K}$; the melt can be supercooled to the glass-transition temperature at approximately $773\ \mathrm{K}$ below which the viscous liquid freezes to a rigid amorphous glass.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 583

glass-like carbon

An agranular non-graphitizable carbon with a very high isotropy of its structural and physical properties and with a very low permeability for liquids and gases. The original surfaces and the fracture surfaces have a pseudo-glassy appearance.
Note:
The often used synonyms 'glassy carbon' and 'vitreous carbon' have been introduced as trademarks and should not be used as terms. From a scientific viewpoint, all synonymous terms suggest a similiarity with the structure of silicate glasses which does not exist in glass-like carbon, except for the pseudo-glassy appearance of the surface. Glass-like carbon cannot be described as amorphous carbon because it consists of two-dimensional structural elements and does not exhibit 'dangling' bonds.
See: agranular carbon

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 490

glass-transition temperature

The temperature at which the viscosity of the glass is $10^{13}\ \mathrm{dPa\ s}$.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 583

global analysis

Method for kinetic analysis of time-resolved emission or absorption data.
Note:
Typical for the analysis of emission (or transient absorption) data. Upon excitation with a particular wavelength, radiant intensity of the emission (or transient absorbance difference) decays are observed as a function of a variable parameter, e.g., the observation wavelength, but otherwise under the same condition. All decays are then analysed together (globally) under the constraint that the lifetimes of the transient species do not vary with the variable parameter, e.g., the observation wavelength in the given example. Lifetime-associated spectra (LAS), also called decay-associated spectra (DAS), are

thus obtained. In the case of transient absorption data, the resulting spectra are often called lifetime-associated difference spectra (LADS).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 349

globular-chain crystal

in polymers

A type of crystal comprised of macromolecules having globular conformations. Globular-chain crystals usually occur with globular proteins.

Source:
Purple Book, p. 84

glove box

An enclosure in which material may be manipulated in isolation from the operator's environment. This manipulation is effected by gauntlet gloves or flexible plastic devices fixed to ports in the walls of the box.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1544

glycals

See: enoses

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

glycans

Synonymous with polysaccharides. Glycans composed of a single type of monosaccharide residue (homopolysaccharide, synonym homoglycan) are named by replacing the ending '-ose' of the sugar by '-an', e.g. mannans, fructans, xylans, arabinans. Dextrans and dextrins belong to the class glucans.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

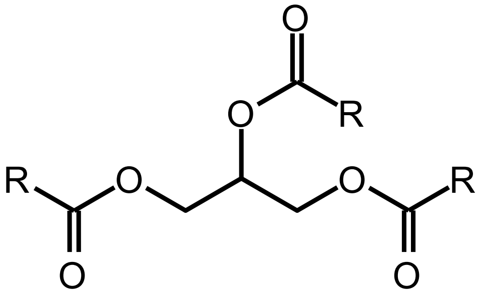
glycaric acids [obsolete]

An obsolescent synonym for aldaric acids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

glycerides

Esters of glycerol (propane-1,2,3-triol) with fatty acids, widely distributed in nature. They are by long-established custom subdivided into triglycerides, 1,2- or 1,3-diglycerides, and 1- or 2-monoglycerides, according to the number and position of acyl groups (not, as one might suppose, the number of glycerol residues). The recommended method for naming individual glycerides is mono-, di- or tri-*O*-acylglycerol, as appropriate.



(a triglyceride)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

See also:
White Book, p. 181

glycerophospholipid

Any derivative of glycerophosphoric acid that contains at least one *O*-acyl, or *O*-alkyl, or *O*-(1-alkenyl) group attached to the glycerol residue.

Source:
White Book, p. 184

glycitols [obsolete]

An obsolescent synonym for alditols.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

glyco-amino-acid

Also contains definition of: glycosyl-amino-acid

A saccharide attached to a single amino acid by any kind of covalent bond. A glycosyl-amino-acid is a compound consisting of saccharide linked through a glycosyl linkage (*O*-, *N*-, or *S*-) to an amino acid.
Note:
The hyphens are needed to avoid implying that the carbohydrate is necessarily linked to the amino group.

Source:
White Book, p. 85

glycoconjugate

A type of compound consisting of carbohydrate units covalently linked with other types of chemical constituent.

Source:
PAC, 1988, *60*, 1389 *(Nomenclature of glycoproteins, glycopeptides and peptidoglycans (Recommendations 1985))* on page 1390
White Book, p. 84

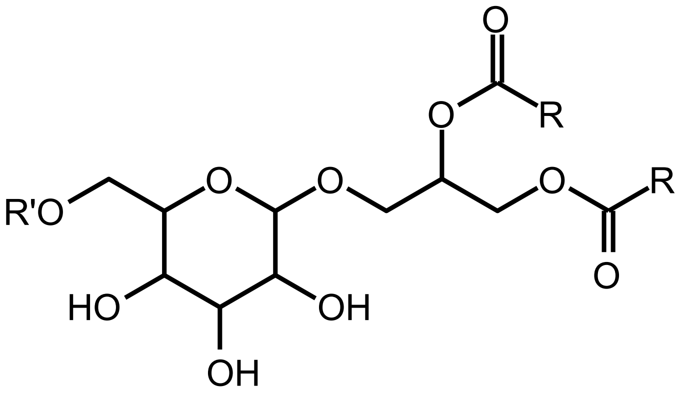
glycoglycerolipid

See: glycolipids

Source:
White Book, p. 129

glycolipids

Naturally occurring 1,2-di-*O*-acylglycerols joined at oxygen 3 by a glycosidic linkage to a carbohydrate part (usually a mono-, di- or tri-saccharide). Some substances classified as bacterial glycolipids have the sugar part acylated by one or more fatty acids and the glycerol part may be absent.



R' = H or glycosyl

See also: glycosides, lipids, lipopolysaccharides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

See also:
White Book, p. 187

glycols

Dihydric alcohols, also known as diols, in which the two hydroxy groups are on different carbon atoms, usually but not necessarily adjacent. E.g. $HOCH_2CH_2OH$ 'ethylene glycol' (ethane-1,2-diol), $HO[CH_2]_4OH$ butane-1,4-diol.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

glyconic acids [obsolete]

An obsolescent synonym for aldonic acids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

glycopeptides (glycoproteins)

Compounds in which a carbohydrate component is linked to a peptide/protein component.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1337

See also:
White Book, p. 84

glycosamines

A term synonymous with amino sugars; now restricted to some trivial names.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

glycosaminoglycan

The carbohydrate units in proteoglycans are polysaccharides that contain amino sugars; these polysaccharides are known as glycosaminoglycans.

Source:
White Book, p. 85

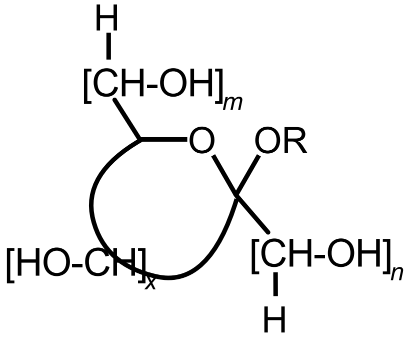
glycoses

A less frequently used term for monosaccharides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

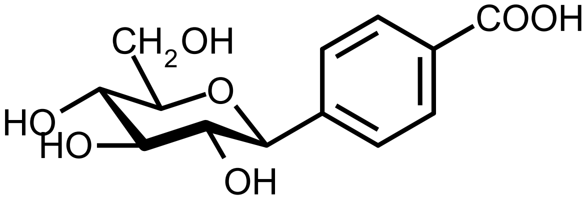
glycosides

Originally mixed acetals resulting from the attachment of a glycosyl group to a non-acyl group RO– (which itself may be derived from a saccharide and chalcogen replacements thereof (RS–, RSe–).



m and n may be 0,1,2,*etc.*; and x usually 2 or 3

The bond between the glycosyl group and the OR group is called a glycosidic bond. By extension, the terms *N*-glycosides and *C*-glycosides are used as class names for glycosylamines and for compounds having a glycosyl group attached to a hydrocarbyl group respectively.



4-β-D-glucopyranosylbenzoic acid, a*C*-glycosyl compound

These terms are misnomers and should not be used. The preferred terms are glycosylamines and *C*-glycosyl compounds, respectively.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338
White Book, p. 136

glycosphingolipid

See: glycolipids

Source:
White Book, p. 187

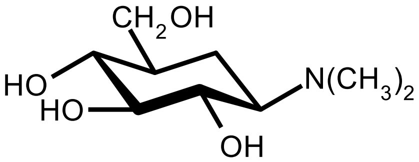
glycosyl group

The structure obtained by removing the hydroxy group from the hemiacetal function of a monosaccharide and, by extension, of a lower oligosaccharide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

glycosylamines

Compounds having a glycosyl group attached to an amino group, NR_2; less elegantly called *N*-glycosides, e.g. *N,N*-dimethyl-β-D-glucopyranosylamine.



See: glycosides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

glycuronic acids [obsolete]

An obsolescent synonym for uronic acids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

See also:
White Book, p. 174

grab sampling

The taking of a sample (often in an evacuated bulb) in a very short time; preferred terms are instantaneous sampling or spot sampling.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2212

gradient

A differential ratio; the change in a quantity such as the mixing ratio of an impurity in air, the temperature of the air, etc., with height or distance.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2192

gradient elution

in chromatography

A procedure in which the composition of the mobile phase is changed continuously or stepwise during the elution process.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 826
Orange Book, p. 93

gradient layer

in chromatography

The chromatographic bed used in thin-layer chromatography in which there is a gradual transition in some property.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 830

See also:
Orange Book, p. 98

gradient packing

Synonymous with gradient layer.

Source:
Orange Book, p. 79

gradientless reactor

in catalysis

Stirred flow or recirculation reactors, characterized ideally by very small concentration and temperature gradients within the catalyst region.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

gradual (sudden) potential-energy surface

These terms relate to the steepness of the energy rise along the reaction path of a potential-energy surface.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 167

graft copolymer

A copolymer that is a graft polymer.
Note:
In the constituent macromolecules of a graft copolymer, adjacent blocks in the main chain or side-chains, or both, are constitutionally different, i.e. adjacent blocks comprise constitutional units derived from different species of monomer or from the same species of monomer but with a different composition or sequence distribution of constitutional units.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2303

graft copolymerization

Polymerization in which a graft copolymer is formed.

Source:
Purple Book, p. 19

graft macromolecule

A macromolecule with one or more species of block connected to the main chain as side chains, these side chains having constitutional or configurational features that differ from those in the main chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2293

graft polymer

A polymer composed of graft macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2303

grafting

in catalysis

See: encapsulation *in catalysis*

Source:
PAC, 1991, *63*, 1227 *(Manual on catalyst characterization (Recommendations 1991))* on page 1230
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 975

grafting

in polymer chemistry

Reaction in which one or more species of block are connected to the main chain of a macromolecule as side-chains having constitutional or configurational features that differ from those in the main chain.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 892

gram

cgs base unit of mass, $\mathrm{g} = 10^{-3}\,\mathrm{kg}$.

Source:
Green Book, 2nd ed., p. 111

Gram stain

A set of two stains that are used to stain (crystal violet and iodine) and counterstain (fuchsin) bacteria. Gram-negative bacteria are completely decolorized after treating the stained bacteria with ethanol or acetone and can be visualized by the counterstain. They have a complex cell wall in which the peptidoglycan layer is covered by lipopolysaccharides in an outer membrane structure. Gram-positive bacteria resist decolorization by ethanol or acetone, they retain the initial Gram stain. They have a cell wall consisting predominantly of peptidoglycan not overlayed by an outer membrane.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 155

granular carbon

The term granular carbon is equivalent to coarse particulate carbon. This is a carbon material consisting of separate particles or grains which are monolithic, on the average larger than about $100\ \mu\text{m}$ in diameter, but smaller than about $1\ \text{cm}$.
Note:
Although limits of size cannot be exactly defined, coke grains obtained by grinding belong to coarse particulate carbon for grain sizes above *ca.* $100\ \mu\text{m}$, or to fine particulate carbon for grain sizes below *ca.* $100\ \mu\text{m}$. Colloidal graphite obtained by grinding of natural graphite is a typical extra fine particulate carbon. Industrial carbon materials (such as electrodes) are made with fillers composed of coarse particulate carbon (coke grains) and fine particulate carbon (flour), and sometimes even colloidal carbon, carbon blacks or soot). They are therefore polygranular materials.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 491

graphene layer

A single carbon layer of the graphite structure, describing its nature by analogy to a polycyclic aromatic hydrocarbon of quasi infinite size.
Note:
Previously, descriptions such as graphite layers, carbon layers or carbon sheets have been used for the term graphene. Because graphite designates that modification of the chemical element carbon, in which planar sheets of carbon atoms, each atom bound to three neighbours in a honeycomb-like structure, are stacked in a three-dimensional regular order, it is not correct to use for a single layer a term which includes the term graphite, which would imply a three-dimensional structure. The term graphene should be used only when the reactions, structural relations or other properties of individual layers are discussed.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 491

graphite

An allotropic form of the element carbon consisting of layers of hexagonally arranged carbon atoms in a planar condensed ring system graphene layers The layers are stacked parallel to each other in a three-dimensional crystalline long-range order. There are two allotropic forms with different stacking arrangements, hexagonal and rhombohedral. The chemical bonds within the layers are covalent with sp^2 hybridization and with a C–C distance of $141.7\ \mathrm{pm}$. The weak bonds between the layers are metallic with a strength comparable to van der Waals bonding only.
Note:
The term graphite is also used often but incorrectly to describe graphite materials, i.e. materials consisting of graphitic carbon made from carbon materials by processing to temperatures greater than $2500\ \mathrm{K}$, even though no perfect graphite structure is present.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 491

graphite fibres

Carbon fibres consisting mostly of synthetic graphite for which three-dimensional crystalline order is confirmed by X-ray diffraction.
Note:
Graphite fibres can be obtained by graphitization heat treatment of carbon fibres if these consist mostly of graphitizable carbon. If the *h,k,l* diffraction lines are difficult to recognize because they are of minor intensity, the mean interlayer spacing $\mathrm{c}/2$ can be used as indication for the presence of a graphitic structure. The $\mathrm{c}/2$ value of $0.34\ \mathrm{nm}$ is generally considered as an upper limit for synthetic graphite.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 492

graphite material

A material consisting essentially of graphitic carbon.
Note:
The use of the term graphite as a short term for material consisting of graphitic carbon is incorrect. The term graphite can only be used in combination with other nouns or clarifying adjectives for special types of graphite materials (graphite electrodes, natural graphite and others). The use of the term graphite without a noun or clarifying adjective should be restricted to the allotropic form of the element carbon.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 492

graphite whiskers

Also contains definition of: carbon whiskers

Thin, approximately cylindrical filaments in which graphene layers are arranged in a scroll-like manner. There is, at least in part, a regular stacking of the layers as in the graphite lattice, giving rise to *h,k,l,* X-ray reflections. The physical properties of graphite whiskers approach, along the cylinder axis, those of graphite.
Note:
If there is, due to misalignment of the layers caused by their bending, no three-dimensional stacking order as in graphite, the term carbon whiskers should be used. Graphite whiskers and carbon whiskers should be distinguished from more disordered filamentous carbon.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 492

graphitic carbon

All varieties of substances consisting of the element carbon in the allotropic form of graphite irrespective of the presence of structural defects.
Note:
The use of the term graphitic carbon is justified if three-dimensional hexagonal crystalline long-range order can be detected in the material by diffraction methods, independent of the volume fraction and the homogeneity of distribution of such crystalline domains. Otherwise, the term non-graphitic carbon should be used.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 493

graphitizable carbon

A non-graphitic carbon which upon graphitization heat treatment converts into graphitic carbon.
Note:
If it is preferred to define the characterizable state of material instead of its behaviour during subsequent treatment, the term 'pregraphitic carbon' could be considered.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 493

graphitization

A solid-state transformation of thermodynamically unstable non-graphitic carbon into graphite by means of heat treatment.
Note:
Graphitization is also used for the transformation of metastable diamond into graphite by heat treatment, as well as in metallurgy for the formation of graphite from thermodynamically unstable

carbides by thermal decomposition at high temperatures. Such uses of the term graphitization are in line with the above definition. The use of the term graphitization to indicate a process of thermal treatment of carbon materials at $T > 2500\ \mathrm{K}$ regardless of any resultant crystallinity is incorrect.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 493

graphitization heat treatment

A process of heat treatment of a non-graphitic carbon industrially performed at temperatures in the range between 2500 and $3300\ \mathrm{K}$, to achieve transformation into graphitic carbon.
Note:
The term graphitization heat treatment does not include information as to the crystallinity achieved by the heat treatment, that is the extent of transformation into graphitic carbon or the degree of graphitization. Only for such a transformation into graphitic carbon should the term graphitization be used. Consequently: the common use of the term graphitization for the heat treatment process only, regardless of the resultant crystallinity, is incorrect and should be avoided.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 493

graphitized carbon

A graphitic carbon with more or less perfect three-dimensional hexagonal crystalline order prepared from non-graphitic carbon by graphitization heat treatment.
Note:
Non-graphitizable carbons do not transform into graphitic carbon on heat treatment at temperatures above $2500\ \mathrm{K}$ and therefore are not graphitized carbons.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 494

gravimetric method

A determination by weight; e.g. in the older method of Cl^- ion determination, a weighed amount of sample is dissolved in water, $AgNO_3$ solution added, AgCl is precipitated, dried and weighed. From the known mass fraction of silver in AgCl, the weights of the initial sample and that of the AgCl precipitated, the percentage of chlorine in the sample can be calculated readily.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2192

gravitational constant

Universal fundamental physical constant in Newton's law of gravitation, $G = 6.672\,59\,(85) \times 10^{-11}\ \mathrm{m^3\ kg^{-1}\ s^{-2}}$.

Source:
CODATA Bull. 1986, *63*, 1

gray

SI derived unit of energy imparted to an element of matter by ionizing radiation divided by the mass of that element (absorbed dose of radiation) equal to one joule per kilogram and admitted for reasons of safeguarding human health, $\mathrm{Gy} = \mathrm{J\ kg^{-1}}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 975

green body

Object formed from a preceramic material prior to pyrolysis.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1811

green coke

Green coke raw coke) is the primary solid carbonization product from high boiling hydrocarbon fractions obtained at temperatures below $900\ \mathrm{K}$. It contains a fraction of matter that can be released as volatiles during subsequent heat treatment at temperatures up to approximately $1600\ \mathrm{K}$. This mass fraction, the so-called volatile matter, is in the case of green coke between 4 and 15 wt.%, but it depends also on the heating rate.
Note:
Raw coke is an equivalent term to green coke although it is now less frequently used. The so-called volatile matter of green coke depends on temperature and time of coking, but also on the method for its determination.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 494

greenhouse effect

in atmospheric chemistry

Heating effect produced by certain gases (e.g. CO_2, O_3, etc.), which by virtue of their characteristic infrared absorption, lower the earth to space transmission of long wavelength radiation but allow transmission of shorter wavelength radiation inward from the sun to the earth.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2192

Grignard reagents

Organomagnesium halides, RMgX, having a carbon–magnesium bond (or their equilibrium mixtures in solution with $R_2Mg + MgX_2$).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

grit

in atmospheric chemistry

Airborne solid particles in the atmosphere which are of natural or manmade origin and which remain in suspension for some time; in the United Kingdom the size of the grit particles is defined as greater than $75\ \mu m$ in diameter (retained on a 200 mesh British Standard sieve).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2193

ground level concentration

in atmospheric chemistry

The concentration of a chemical species, normally a pollutant, in air; usually measured at a specific height above the ground.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2181

ground level inversion

in atmospheric chemistry

The inversion of the normal temperature gradient in the atmosphere; the temperature of the air increases with increasing height of the air above the ground. This leads to poor mixing of gases released below the inversion.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2193

ground state

The state of lowest Gibbs energy of a system.
See also: excited state

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1118

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2245
Orange Book, p. 227

group

A defined linked collection of atoms or a single atom within a molecular entity. This use of the term in physical organic and general chemistry is less restrictive than the definition adopted for the purpose of nomenclature of organic compounds.
See also: characteristic group *in organic nomenclature*, principal group *in organic nomenclature*, substituent

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1118

See also:
Blue Book, p. 82
Blue Book, p. 85

group electronegativity

Synonymous with substituent electronegativity.
See: electronegativity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169

group preconcentration

in trace analysis

An operation (process) as a result of which several microcomponents are isolated in one step. This may be achieved in one of two ways, by transportation either of the matrix or of the microcomponents into a second phase. The first method is widely used in the analysis of relatively simple substances and materials.

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1198

growth curve

of activity

Curve giving the activity of a radioactive nuclide as a function of time and showing the increase of the activity through the decay of the precursor or as a result of activation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

growth rate

in biotechnology

The measure (h^{-1}, d^{-1}) of the rate of growth or multiplication of an organism or a culture, usually expressed as specific growth rate (the increase of mass or cell number per time unit referred to the unit of mass, $\frac{\mathrm{d}(\ln X)}{\mathrm{d}t}$).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

Grunwald–Winstein equation

The linear free energy relation:

$$\log_{10}\left(\frac{k_{\mathrm{s}}}{k_0}\right) = m\,Y$$

expressing the dependence of the rate of solvolysis of a substrate on ionizing power of the solvent. The rate constant k_0 applies to the reference solvent (ethanol–water, 80:20, v/v) and k_{s} to the solvent **s**, both at 25 °C. The parameter m is characteristic of the substrate and is assigned the value unity for *tert*-butyl chloride. The value Y is intended to be a quantitative measure of the ionizing power of the solvents. The equation was later extended to the form:

$$\log_{10}\left(\frac{k_{\mathrm{s}}}{k_0}\right) = m\,Y + l\,N$$

where N is the nucleophilicity of the solvent and l its susceptibility parameter. The equation has also been applied to reactions other than solvolysis.

See also: Dimroth–Reichardt E_T parameter, polarity, Z-value

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1118

guest

An organic or inorganic ion or molecule that occupies a cavity, cleft or pocket within the molecular structure of a host molecular entity and forms a complex with it or that is trapped in a cavity within the crystal structure of a host.
See also: crown, cryptand, inclusion compound

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1118

Guinier plot

A diagrammatic representation of data on scattering from large particles, obtained at different angles but at the same concentration, constructed by plotting $\log_{10}\Delta R(\theta)$ or $\log_{10}P(\theta)$ *versus* $\left(\sin\frac{\theta}{2}\right)^2$ or q^2 and (usually) used for the evaluation of the radius of gyration. $\Delta R(\theta)$ is the excess Rayleigh ratio, $P(\theta)$ the particle scattering function, θ the scattering angle and q the length of the scattering vector.

Source:
Purple Book, p. 67

gustiness

in atmospheric chemistry

Intensity of turbulence; the ratio of the root mean square of wind velocity fluctuations to the mean wind velocity.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2193

Haber–Weiss reaction

The Haber–Weiss cycle consists of the following two reactions:

$H_2O_2 + OH^{\cdot} \longrightarrow H_2O + O_2^{-} + H^{+}$ and

$H_2O_2 + O_2^{-} \longrightarrow O_2 + OH^{-} + OH^{\cdot}$

The second reaction achieved notoriety as a possible source of hydroxyl radicals. However, it has a negligible rate constant. It is believed that iron(III) complexes can catalyse this reaction: first, Fe(III) is reduced by superoxide, followed by oxidation by dihydrogen peroxide.
See also: Fenton reaction

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1277

haem

An alternative spelling for heme.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

halato-telechelic polymer

Also contains definition of: halatopolymer

Polymer composed of linear macromolecules having ionic or ionizable end-groups.
Notes:

1. The term halato-telechelic polymer is used to denote a polymer composed of macromolecules having stable (long-lived) ionic or ionizable groups, such as carboxylate or quaternary ammonium groups, as chain ends. It should not be used to describe a polymer composed of macromolecules having chain ends that are transient intermediates in ionic polymerizations initiated by difunctional initiators.
2. The term halatopolymer is used for a linear polymer formed by the coupling of halato-telechelic polymer molecules, for example, for the linear polymer formed by the coupling of carboxylate end-groups with divalent metal cations.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2070

half life, $t_{1/2}$

For a given reaction the half life $t_{1/2}$ of a reactant is the time required for its concentration to reach a value that is the arithmetic mean of its initial and final (equilibrium) values. For a reactant that is entirely consumed it is the time taken for the reactant concentration to fall to one half its initial value:
The half life of a reaction has meaning only in special cases:

1. For a first-order reaction, the half life of the reactant may be called the half life of the reaction.
2. For a reaction involving more than one reactant, with the concentrations of the reactants in their stoichiometric ratios, the half life of each reactant is the same, and may be called the half life of the reaction.

If the concentrations of reactants are not in their stoichiometric ratios, there are different half lives for different reactants, and one cannot speak of the half life of the reaction.
See also: lifetime

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 167

PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1119
Green Book, 2nd ed., p. 55
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 975

half life

Synonym: radioactive half life

of a radionuclide

For a single radioactive decay process, the time required for the activity to decrease to half its value by that process.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

half thickness

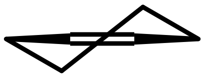
in radiochemistry

The thickness of a specified substance which, when introduced into the path of a given beam of radiation, reduces the value of a specified radiation quantity by one half.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

half-chair

The conformation of a six-membered ring structure in which four contiguous atoms are in a plane and the other two atoms lie on opposite sides of the plane.



See also: chair, boat, twist

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2209

half-life, $\tau_{1/2}$,

of a transient entity

Time needed for a concentration of the entity to decrease to $1/2$ of its original value.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 349

half-life, $T_{1/2}$,

of a photochromic system

Time necessary for thermal bleaching to half of the absorbance of the coloured form of a photochromic compound at a specific wavelength during one cycle.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 349

half-peak potential

In linear-sweep voltammetry, triangular-wave voltammetry, cyclic triangular-wave voltammetry, and similar techniques, the potential of the indicator electrode at which the difference between the total current and the residual current is equal to one-half of the peak current. This potential is attained in the interval in which the rate of the charge-transfer process, and hence the (absolute value of the) current, increase monotonically with time.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1502

half-wave potential

The potential of a polarographic or voltammetric indicator electrode at the point, on the rising part of a polarographic or voltammetric wave, where the difference between the total current and the residual current is equal to one-half of the limiting current. The quarter-wave potential, the three-quarter-wave potential, etc., may be similarly defined.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1502

half-width

of a band

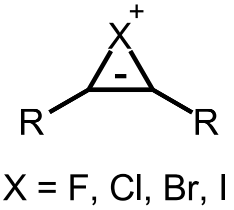
The full width of a spectral band at a height equal to half of the height at the band maximum. Also known as full width at half maximum (FWHM). The dimension of band width should be either inverse length (wavenumbers) or inverse time (frequencies) so that the values give an indication of the energies. Note the hyphen in half-width. Half bandwidth has the meaning of half-width at half maximum.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2245

See also:
Orange Book, p. 226

halirenium ions

Cyclic cations having the structure:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

halochromism

The colour change which occurs on addition of acid (or base, or a salt) to a solution of a compound. A chemical reaction (e.g. ion formation) transforms a colourless compound into a coloured one.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1119

haloforms

Trihalomethanes CHX_3.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

halohydrins

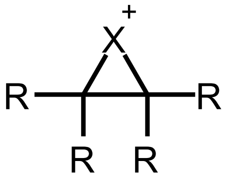
A traditional term for alcohols substituted by a halogen atom at a saturated carbon atom otherwise bearing only hydrogen or hydrocarbyl groups (usually used to mean β-halo alcohols). E.g. $BrCH_2CH_2OH$ 'ethylene bromohydrin' (2-bromoethanol), $ClCH_2CH_2CH_2OH$ 'trimethylene chlorohydrin' (3-chloro-propan-1-ol), $PhCH(OH)CH_2Cl$ 'styrene chlorohydrin' (2-chloro-1-phenylethanol).

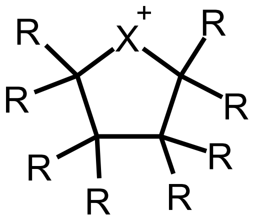
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1338

halonium ions

Also contains definitions of: bromonium ions, chloronium ions, iodonium ions

Ions of the form R_2X^+, where X is any halogen ($X = Br^+$, bromonium ions; $X = Cl^+$, chloronium ions; $X = F^+$, fluoronium ions; $X = I^+$, iodonium ions). They may be open-chain or cyclic.





Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

halophiles

Organisms which require a minimum concentration of sodium chloride in their environment (cf. extremophiles).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

hamiltonian operator $\hat{H}$

Quantum mechanical operator of total energy.

Source:
Green Book, 2nd ed., p. 16

Hammett equation (Hammett relation)

The equation in the form:

$$\log_{10}\left(\frac{k}{k_0}\right) = \rho\,\sigma$$

or

$$\log_{10}\left(\frac{K}{K_0}\right) = \rho\,\sigma$$

applied to the influence of *meta*- or *para*-substituents X on the reactivity of the functional group Y in the benzene derivative *m*- or *p*-XC_6H_4Y. k or K is the rate or equilibrium constant, respectively, for the given reaction of *m*- or *p*-XC_6H_4Y; k_0 or K_0 refers to the reaction of C_6H_5Y, i.e. X = H; is the substituent constant characteristic of *m*- or *p*-X: is the reaction constant characteristic of the given reaction of Y. The equation is often encountered in a form with $\log_{10}k_0$ or $\log_{10}K_0$ written as a separate term on the right hand side, e.g.

$$\log_{10}k = \rho\,\sigma + \log_{10}k_0$$

or

$$\log_{10}K = \rho\,\sigma + \log_{10}K_0$$

It then signifies the intercept corresponding to X = H in a regression of $\log_{10}k$ or $\log_{10}K$ on σ.
See also: ρ-value, σ-constant, Taft equation, Yukawa-Tsuno equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1119

Hammond principle (Hammond postulate)

Also contains definition of: Leffler's assumption

The hypothesis that, when a transition state leading to an unstable reaction intermediate (or product) has nearly the same energy as that intermediate, the two are interconverted with only a small reorganization of molecular structure. Essentially the same idea is sometimes referred to as 'Leffler's assumption', namely, that the transition state bears the greater resemblance to the less stable species (reactant or reaction intermediate/product). Many text books and physical organic chemists, however, express the idea in Leffler's form, but attribute it to Hammond. As a corollary, it follows that a factor stabilizing a reaction intermediate will also stabilize the transition state leading to that intermediate. The acronym 'Bemahapothle' (Bell, Marcus, Hammond, Polanyi, Thornton, Leffler) is sometimes used in recognition of the principal contributors towards expansion of the original idea of the Hammond postulate.
See also: More O'Ferrall-Jencks diagram

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1119

Hammond–Herkstroeter plot

See: energy transfer plot

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2245

handedness

This term has been used in two ways, either chirality or chirality sense

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2209

Hansch analysis

Hansch analysis is the investigation of the quantitative relationship between the biological activity of a series of compounds and their physicochemical substituent or global parameters representing hydrophobic, electronic, steric and other effects using multiple regression correlation methodology.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1144

Hansch constant

A measure of the capability of a solute for hydrophobic lipophilic interaction based on the partition coefficient P for distribution of the solute between octan-1-ol and water. The most general way of applying P in correlation analysis, QSAR, etc. is as log P, but the behaviour of substituted benzene derivatives may be quantified by a substituent constant scale, π, which is defined in a way analogous to the Hammett σ scale. There are various scales, depending on the substrate series used as reference.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1119

Hantzsch–Widman name

A name for a heteromonocyclic parent hydride having no more than ten ring members formed by the citation of 'a' prefixes denoting the heteroatoms followed by an ending (the 'stem') defining the size of the ring.

Source:
Blue Book (Guide), p. 14

hapten

A low-molecular weight molecule which contains an antigenic determinant but which is not itself antigenic unless complexed with an anitgenic carrier. Examples of haptens are dinitrophenols, phosphorylcholine and dextran.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

hapto

See: η or hapto

hard acid

Also contains definition of: soft acid

A Lewis acid with an acceptor centre of low polarizability. Other things being approximately equal, complexes of hard acids and bases or soft acids and bases have an added stabilization (sometimes called 'HSAB' rule). For example the hard O- (or N-) bases are preferred to their S- (or P-) analogues by hard acids. Conversely a soft acid possesses an acceptor centre of high polarizability and exhibits the reverse preference for coordination of a soft base. These preferences are not defined in a quantitative sense.
See also: class (a) metal ion

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120

hard amorphous carbon films

A synonym for diamond-like carbon films

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 494

hard base

Also contains definition of: soft base

A Lewis base with a donor centre (e.g. an oxygen atom) of low polarizability the converse applies to soft bases.
See also: hard acid

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120

hard-segment phase domain

Phase domain of microscopic or smaller size, usually in a block, graft, or segmented copolymer, comprising essentially those segments of the polymer that are rigid and capable of forming strong intermolecular interactions.
Note:
Hard-segment phase domains are typically of $2–15$ nm linear size.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2002

hard-sphere collision cross section

See: reaction probability

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 766

harmonic approximation

The approximation of the full nuclear potential of a molecular system in its equilibrium geometry and in the vicinity of the respective minimum on the potential energy surface by the function

$$V = \frac{1}{2} \sum_{i,j=1}^{3N} \frac{\partial^2 V}{\partial q_i \partial q_j}$$

where q_i are mass-weighted cartesian displacements of nuclei relative to their equilibrium positions. The approximation allows one to describe vibrational motion in terms of independent vibrational modes (normal modes) each of which is governed by a simple one-dimensional harmonic potential.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1941

harmonic frequency generation

Production of coherent radiation of frequency $k\nu$ ($k = 2, 3, ...$) from coherent radiation of frequency. In general, this effect is obtained through the interaction of laser light with a suitable optical medium with non-linear polarizability. The case $k = 2$ is referred to as frequency doubling, $k = 3$ is frequency tripling and $k = 4$ is frequency quadrupling. Even higher integer values of k are possible.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2245

harmonic mean

The number of observations, divided by the sum of reciprocals of the observations. Symbol: $\bar{x}_\mathrm{h}$. It can be calculated with the formula:

$$\bar{x}_\mathrm{h} = \frac{n}{\sum x_j^{-1}}$$

Note:
As in the case of the geometric mean, this quantity is sometimes directly (but inappropriately) calculated, for example, when evaluating kinetic analytical results where the reaction time is inversely proportional to concentration.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 602

harpoon mechanism

Reaction sequence (thermal or photoinduced) between neutral molecular or atomic entities in which long-range electron transfer is followed by a considerable reduction of the distance between donor and acceptor sites as a result of the electrostatic attraction in the ion pair created.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2245

hartree

Atomic unit of energy, $E_\mathrm{h} \approx 4.359\ 7482\ (26) \times 10^{-18}$ J.

Source:
Green Book, 2nd ed., p. 76

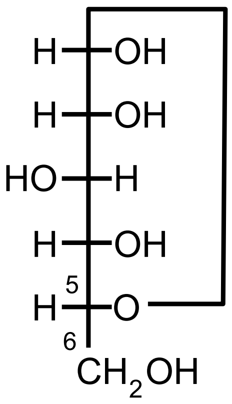
Hartree energy

Atomic fundamental physical constant used as atomic unit of energy: $\mathrm{E_h} = \frac{\hbar^2}{m_\mathrm{e}\, a_0^{\,2}} = 4.359\ 7482\ (26) \times 10^{-18}$ J, where $\hbar$ is the Planck constant divided by $2\,\pi$, m_e the electron rest mass and a_0 the Bohr radius.

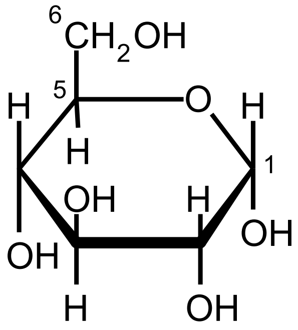
Source:
CODATA Bull. 1986, *63*, 1

Haworth representation

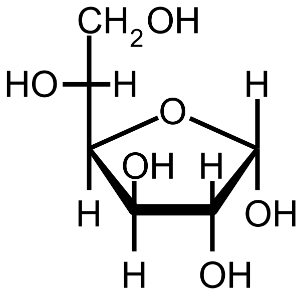
The Haworth representation of the cyclic forms of monosaccharides can be derived from the Fischer projection, as follows. The monosaccharide is depicted with the carbon-chain horizontal and in the plane of the paper, the potential carbonyl group being to the right. The oxygen bridge is then depicted as being formed behind the plane of the paper. The heterocyclic ring is therefore located in a plane approximately perpendicular to the plane of the paper and the groups attached to the carbon atoms of that ring are above and below the ring. The carbon atoms of the ring are not shown. Groups that appear to the right of the vertical chain in the Fischer projection (structures A, D) then appear below the plane of the ring in the Haworth representation (structures B, C, E). However, at the asymmetric carbon atom (C-5 in A; C-4 in D) involved via oxygen in ring formation with the carbon atom of the carbonyl group a formal double inversion must be envisaged to obtain the correct Haworth representation. In the pyranose forms of D-aldohexoses C-6 will always be above the plane, In the furanose forms of D-aldohexoses the position of C-6 will depend on the configuration at C-4; it will, for example, be above the plane in D-glucofuranoses (e.g. C) but below the plane in D-galactofuranoses (e.g. E).



(A)



(B)



(C)

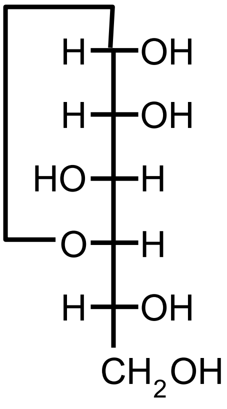
α-D-glucopyranose

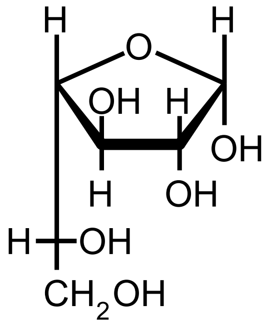
α-D-glucofuranose

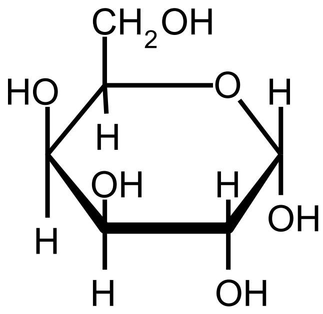
(Fischer)

(Haworth)

(Haworth)







(D) (E) (F)

α-D-galactofuranose α-D-galactopyranose

(Fischer) (Haworth) (Haworth)

Source:
White Book, p. 128

hazard

Set of inherent properties of a substance, mixture of substances, or a process involving substances that, under production, usage, or disposal conditions, make it capable of causing adverse effects to organisms or the environment, depending on the degree of exposure; in other words, it is a source of danger.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1054

haze horizon

in atmospheric chemistry

The top of a haze layer which is confined by a low-level temperature inversion so that it gives the appearance of the horizon which it may obscure.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2193

haze

in atmospheric chemistry

A state of reduced visibility ($1 - 2\ \mathrm{km}$) resulting from the increased light scatter due to the presence of fine dust or aerosol particles (H_2SO_4, NH_4HSO_4, products of the ozone-terpene reactions, etc.).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2193

health surveillance

The procedure for effects of work on the health of employees.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1023

heat, q, Q

Energy transferred from a hotter to a cooler body due to a temperature gradient.

Source:
Green Book, 2nd ed., p. 48

heat capacity, C

Heat brought to a system to increase its temperature divided by that temperature increase. At constant volume $C_V = \left(\frac{\partial U}{\partial T}\right)_V$ at constant pressure $C_p = \left(\frac{\partial H}{\partial T}\right)_p$, where U is the internal energy and H the enthalpy of the system.

Source:
Green Book, 2nd ed., p. 48
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 975

heat capacity of activation, $\Delta^{\ddagger}C_p^{\mathrm{o}}$

A quantity related to the temperature coefficient of $\Delta^{\ddagger}H$ (enthalpy of activation) and $\Delta^{\ddagger}S$ (entropy of activation) according to the equations:

$$\Delta^{\ddagger}C_p = \left(\frac{\partial \Delta^{\ddagger}H}{\partial T}\right)_p = T\left(\frac{\partial \Delta^{\ddagger}S}{\partial T}\right)_p$$

If the rate constant is expressible in the form

$$\ln k = \frac{a}{T} + b + c\,\ln T + \mathrm{d}T,$$

then:

$$\Delta^{\ddagger}C_p = (c-1)\,R + 2\,\mathrm{d}(R\,T)$$

SI unit: J mol^{-1} K^{-1}.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 168

heat flux, J_q

Heat transferred through a cross section perpendicular to the flow in a small time interval divided by that time interval and the cross sectional area.
See also: flux

Source:
Green Book, 2nd ed., p. 65

heavy atom effect

The enhancement of the rate of a spin-forbidden process by the presence of an atom of high atomic number, which is either part of, or external to, the excited molecular entity. Mechanistically, it responds to a spin-orbit coupling enhancement produced by a heavy atom.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2245

heavy atom isotope effect

An isotope effect due to isotopes other than those of hydrogen.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1130

heavy water

Water containing a significant fraction (up to 100 per cent) of deuterium in the form of D_2O or HDO.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1544

hecto

SI prefix for 10^2 (symbol: h).

Source:
Green Book, 2nd ed., p. 74

height equivalent to a theoretical plate

Acronym: h.e.t.p.

in chromatography

The column length divided by the theoretical plate number.

Source:
Orange Book, p. 108

height equivalent to an effective theoretical plate

Acronym: h.e.e.t.p.

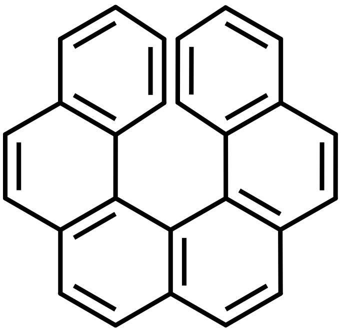
in chromatography

The column length divided by the effective theoretical plate number.

Source:
Orange Book, p. 108

helicenes

ortho-Fused polycyclic aromatic or heteroaromatic compounds in which all rings (minimum five) are angularly arranged so as to give helically shaped molecules, which are thus chiral, e.g. hexahelicene.

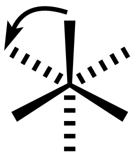


Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

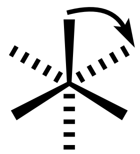
helicity

Also contains definitions of: *M*, *P*, *M*

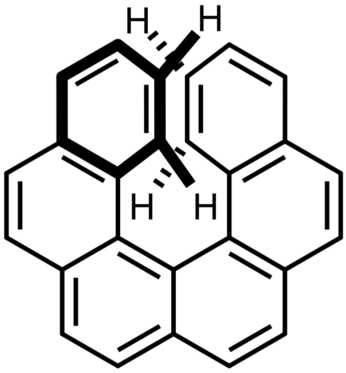
The chirality of a helical, propeller or screw-shaped molecular entity. A right-handed helix is described as *P* (or plus), a left-handed one as *M* (or minus).



M or Λ



P or Δ



(*M*)-hexahelicene

The application of this system to the description of conformations considers the torsion angle between two specified (fiducial) groups that are attached to the atoms linked by that bond. The sign of the smaller torsion angle between the fiducial groups defines the chirality sense of the helix. Rules for the selection of fiducial groups according to priority are given by R.S. Cahn, C.K. Ingold and V. Prelog, *Angew. Chem. 78*, 413-447 (1966), *Angew. Chem. Internat. Ed. Eng. 5*, 385-415, 511 (1966).
See also: axial chirality, Δ (delta), Λ (lambda)

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2209

heliochromism

Applied to photochromic compounds possessing a high efficiency for colouring with near-ultraviolet radiation and a low efficiency for bleaching with visible radiation, but a moderate efficiency for thermal fading at ambient temperature. These compounds are activated by unfiltered sunlight and deactivated under diffuse daylight conditions, therefore being suitable for sun-lens applications.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 350

helion

Nucleus of the ^{3}He atom.

Source:
Green Book, 2nd ed., p. 93

helium dead-space

in colloid and surface chemistry

The position of the Gibbs surface is often defined experimentally as that surface which encloses the volume of space from which the solid excludes helium gas (the so-called helium dead-space), and is associated with the assumptions that the volume of the solid is unaffected by the adsorption of component **i**, and that helium is not adsorbed by the solid. This requires that the measurement of the helium dead-space be made at a sufficiently high temperature.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 595

helium ionization detector

in gas chromatography

A weak beta source and a high potential raise the helium atom of the carrier gas to a metastable state. All other substances having an ionization potential lower than $18\ \mathrm{eV}$ are ionized, and the current that results is used to measure the components. The detector is usually employed to measure inorganic compounds at concentrations between 0.1 and $10\ \mathrm{ppmv}$. It has a linear range of about 10^{2} but is somewhat unstable and requires great care to ensure the helium purity and to eliminate all leaks in the system.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

helium–cadmium laser

Synonym: cadmium–helium laser

A continuous wave laser emitting mainly at 325.0 and $441.6\ \mathrm{nm}$ from singly ionized cadmium.
See: gas lasers

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

helium–neon laser

A continuous wave laser emitting mainly at $632.8\ \mathrm{nm}$, $1152.3\ \mathrm{nm}$, and $3391.3\ \mathrm{nm}$ from excited neutral Ne atoms.
See: gas lasers

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

helix

The molecular conformation of a spiral nature, generated by regularly repeating rotations around the backbone bonds of a macromolecule.

Source:
Purple Book, p. 78

helix residue

in a polymer

The smallest set of one or more successive configurational base units that generates the whole chain through helical symmetry.

Source:
Purple Book, p. 79

helix sense

The right-handed sense of a helix traces out a clockwise rotation moving away from the observer; the left-handed sense of a helix traces out a counterclockwise rotation moving away from the observer, e.g. the ...$\mathrm{TG^+TG^+TG^+}$ ... helix of isotactic poly(propylene) is left-handed.

Source:
Purple Book, p. 43

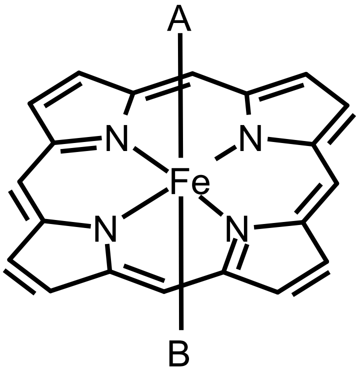
Helmholtz energy (function), *A*

Internal energy minus the product of thermodynamic temperature and entropy. It was formerly called free energy.

Source:
Green Book, 2nd ed., p. 48

hemes (heme derivatives)

Complexes consisting of an iron ion coordinated to a porphyrin acting as a tetradentate ligand, and to one or two axial ligands.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

See also:
White Book, p. 311
White Book, p. 316

hemiacetals

Compounds having the general formula $R_2C(OH)OR'$ ($R' \neq H$).
See also: lactols, hemiketals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

hemiaminals

α-Amino alcohols, improperly called carbinolamines (the adducts of ammonia, or of primary or secondary amines to the carbonyl group of aldehydes and ketones) $R_2C(OH)NR_2$. Compounds of structure $R_2C(OR')NR_2$ ($R \neq H$) are hemiaminal ethers, or α-amino ethers.
See: alcohols, aminals, ethers

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

hemiketals

Hemiacetals having the structure $R_2C(OH)OR$ ($R \neq H$), derived from ketones by formal addition of an alcohol to the carbonyl group. This term, once abandoned, has been reinstated as a subclass of hemiacetals.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

hemileptic [obsolete]

See: homoleptic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120

hemins

Chloro(porphyrinato)iron(III) complexes.
See also: hemes (heme derivatives)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

See also:
White Book, p. 316

hemochromes

Iron–porphyrin complexes, having one or two basic ligands (e.g. piperidine, amines).
See also: hemes (heme derivatives)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

See also:
White Book, p. 316

hemodialysis

Dialysis process in which undesired metabolites and toxic by-products, such as urea and creatine, are removed from blood.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1487

hemoglobins

Heme derivatives having a protein chain as axial ligand.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

Henderson–Hasselbalch equation

An equation of the form:

$$\mathrm{pH} = \mathrm{p}K_{\mathrm{a}} - \log_{10}\left(\frac{[\mathrm{HA}]}{[\mathrm{A}^{-}]}\right)$$

for the calculation of the pH of solutions where the ratio $\frac{[\mathrm{HA}]}{[\mathrm{A}^{-}]}$ is known.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120

henry

SI derived unit of inductance, $\mathrm{H} = \mathrm{V\ A^{-1}\ s} = \mathrm{m^2\ kg\ s^{-2}\ A^{-2}}$.

Source:
Green Book, 2nd ed., p. 72

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 975

Henry's law

Also contains definition of: Raoult's law

The partial pressure (fugacity) of a solute (B) in a solution is directly proportional to the rational chemical activity (a_x) of the solute; this relationship is called Henry's law:

$$p_{\mathrm{B}} = \frac{a_{x,\mathrm{B}}}{\alpha^{\infty}_{x,\mathrm{B}}}$$

where $\alpha^{\infty}_{x,\mathrm{B}}$ is the rational solubility coefficient for infinite dilution, i.e. for pure solvent. For the solvent (A) the relationship is called Raoult's law, and the proportionality factor is the fugacity of the pure solvent, $\tilde{p}^{*}_{\mathrm{A}}$:

$$p_{\mathrm{A}} = \tilde{p}^{*}_{\mathrm{A}}\, a_{\mathrm{A}}$$

Source:
PAC, 1984, *56*, 567 *(Physicochemical quantities and units in clinical chemistry with special emphasis on activities and activity coefficients (Recommendations 1983))* on page 571

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2193
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 544

Herkstroeter plot

See: energy transfer plot

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

hertz

SI derived unit of frequency equal to one cycle per second, $\mathrm{Hz} = \mathrm{s}^{-1}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 976

Herz compounds

1,2λ^4,3-Benzodithiazolium chlorides (formed in the reaction of aniline and derivatives thereof with disulfur dichloride).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1339

hetarenes

Synonymous with heteroarenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

hetaryl groups

Synonymous with heteroaryl groups.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

hetarynes

Synonymous with heteroarynes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

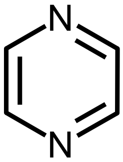
heteroalkenes

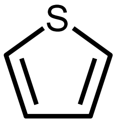
Analogues of alkenes in which a doubly bonded carbon atom is replaced by a heteroatom, e.g. $H_2Si{=}CH_2$ methylidenesilane (silene less preferred), $MeN{=}CH_2$ *N*-methylmethanimine.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

heteroarenes

Heterocyclic compounds formally derived from arenes by replacement of one or more methine (–C=) and/or vinylene (–CH=CH–) groups by trivalent or divalent heteroatoms, respectively, in such a way as to maintain the continuous π-electron system characteristic of aromatic systems and a number of out-of-plane π-electrons corresponding to the Hückel rule ($4\,n + 2$); an alternative term is hetarenes.

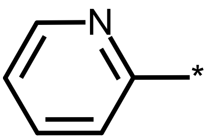




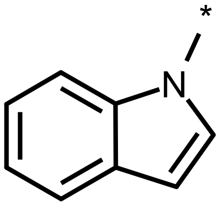
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

heteroaryl groups

The class of heterocyclyl groups derived from heteroarenes by removal of a hydrogen atom from any ring atom; an alternative term is hetaryl. E.g.



2-pyridyl (pyridin-2-yl)

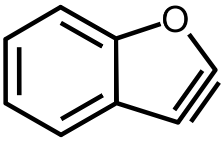


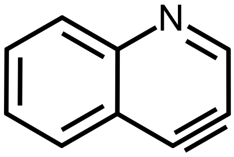
indol-1-yl

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

heteroarynes

Compounds derived from heteroarenes by replacement of a formal carbon-carbon double bond by a formal triple bond (with loss of two hydrogen atoms). Also known as hetarynes and as 1,2-didehydroheteroarenes. E.g.





See: arynes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

heterobimetallic complex

A metal complex having two different metal atoms.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120

heterochain polymer

A class of polymer in which the main chain is constructed from atoms of two or more elements. Heterochain polymers are named by placing the names or symbols of all the elements in the main chain, immediately before the expresssion '-chain polymer', e.g. (oxygen, carbon)-chain polymer or (O, C)-chain polymer; (oxygen, nitrogen, carbon)-chain polymer or (O, N, C)-chain polymer.

Source:
Purple Book, p. 146

heteroconjugation

1. [obsolete] Association between a base and the conjugate acid of a different base through a hydrogen bond (B' ... HB$^+$ or A'H ... A$^-$). The term has its origin in the conjugate acid–base pair and is in no way related to conjugation of orbitals Heteroassociation is a more appropriate term.
2. [obsolete] Some authors refer to conjugated systems containing a heteroatom, e.g. pyridine, as 'heteroconjugated systems'. This usage is discouraged since it inappropriately suggests an analogy to homoconjugation, and conflicts with the currently accepted definition of that term.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120

heterocumulenes

Cumulenes in which one or more carbon atoms of the cumulative bond system have been replaced by heteroatoms. E.g. O=C=C=C=O, but not CH_2=C=O, ketene, nor O=C=O, carbon dioxide, which are heteroallenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

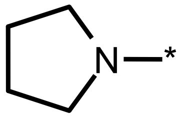
heterocyclic compounds

Cyclic compounds having as ring members atoms of at least two different elements, e.g. quinoline, 1,2-thiazole, bicyclo[3.3.1]tetrasiloxane.
See: homocyclic compounds, carbocyclic compounds

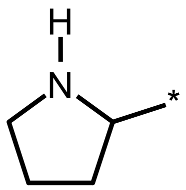
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

heterocyclyl groups

Univalent groups formed by removing a hydrogen atom from any ring atom of a heterocyclic compound. E.g.



pyrrolidin-1-yl



pyrrolidin-2-yl

See: organyl

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

heterodetic cyclic peptide

A peptide consisting only of amino-acid residues, but in which the linkages forming the ring are not solely eupeptide bonds; one or more is an isopeptide, disulfide, ester, or other bond.

Source:
White Book, p. 59

heterodisperse

Describes a colloidal system in which all the particles are of different sizes.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

heteroexcimer

Synonymous with exciplex.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

heterogeneous diffusion rate constant

in electrochemistry

Defined by the equation:

$$k_{\mathrm{d}} = \frac{I_{\mathrm{l}}}{n\,F\,c\,A}$$

where the limiting current I_{l} is assumed to be due to the diffusion species of concentration c and of diffusion coefficient D. n is the charge number of the cell reaction written so that the stoichiometric coefficient of this species is unity. A is usually taken as the geometric area of the electrode, and F is the Faraday constant.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 513

heterogeneous nucleation

See: embryo, nucleation

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

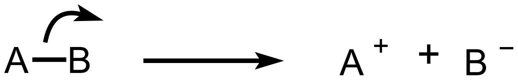
heteroleptic

Transition metal or Main Group compounds having more than one type of ligand.
See also: homoleptic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120

heterolysis (heterolytic)

The cleavage of a covalent bond so that both bonding electrons remain with one of the two fragments between which the bond is broken, e.g.



Heterolytic bond fission is a feature of many bimolecular reactions in solution (e.g. electrophilic substitution, nucleophilic substitution).
See also: homolysis, heterolytic bond-dissociation energy

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1120

heterolytic bond-dissociation energy

The energy required to break a given bond of some specific compound by heterolysis. For the dissociation of a neutral molecule AB in the gas phase into A^+ and B^- the heterolytic bond-dissociation energy $\mathrm{D}(A^+\,B^-)$ is the sum of the bond dissociation energy, $D(\mathrm{A–B})$, and the adiabatic ionization energy of the radical $A^{\cdot}$ minus the electron affinity of the radical $B^{\cdot}$.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1121

heterolytic dissociative adsorption

Relates in the usual sense to the formal nature of the cleavage of a single bond. If in the bond of the adsorptive A:B, A or B retains the electron pair, the adsorption is heterolytic dissociative adsorption.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

heteropolysaccharide (heteroglycan)

The class name for polysaccharides composed of two or more different kinds of monomeric units (i.e. monosaccharides).

Source:
White Book, p. 174

heterotactic polymer

See: triads

Source:
Purple Book, p. 40

heterotactic triads

in polymers

See: triads

Source:
Purple Book, p. 40

heterotopic

See: stereoheterotopic

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

heterotrophic (organisms)

Descriptive of organisms which are not able to synthesize cell components from carbon dioxide as sole carbon source. Heterotrophic organisms use preformed oxidizable organic substrates such as glucose as carbon and energy sources.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

hexagonal graphite

The thermodynamically stable form of graphite with an ABAB stacking sequence of the graphene layers. The exact crystallographic description of this allotropic form is given by the space group $d_{6h}^{4} - P6_{3}/\mathrm{mmc}$ (unit cell constants: $a = 245.6\ \mathrm{pm}$, $c = 670.8\ \mathrm{pm}$). Hexagonal graphite is thermodynamically stable below approximately $2600\ \mathrm{K}$ and $6\ \mathrm{GPa}$.
Note:
The use of the term graphite instead of the more exact term hexagonal graphite may be tolerated in view of the minor importance of rhombohedral graphite, the other allotropic form.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 494

hexahedro-

in inorganic nomenclature

An affix used in names to denote eight atoms bound into a hexahedron (e.g. cube).

Source:
Red Book, p. 245
Blue Book, p. 464

hexaprismo-

in inorganic nomenclature

An affix used in names to denote twelve atoms bound into a hexagonal prism.

Source:
Red Book, p. 245
Blue Book, p. 464

high resolution energy loss spectroscopy (HRELS)

See: reflection electron energy loss spectroscopy (REELS)

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2025

high-pressure graphitization

A term which refers to the solid-state transformation of non-graphitic carbon into graphite by heat treatment under elevated pressure (e.g. 100 to $1000\ \mathrm{MPa}$) so that a definitely higher degree of graphitization is achieved at lower temperature and/or for a shorter heat treatment time than in heat treatment of the same non-graphitic material at atmospheric pressure.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 495

high-pressure mercury lamp (arc)

Radiation source containing mercury at a pressure of *ca.* $8\ \mathrm{MPa}$ (*ca.* $80\ \mathrm{bar}$) or higher which emits lines over a background continuum between about 200 and $1400\ \mathrm{nm}$.
See: lamp

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

higher-order transition

Synonym: smooth transition

A general term used to describe a transition in which the first and second derivatives of the molar Gibbs energy or molar Helmholtz energy (or chemical potential) with respect to temperature and pressure are continuous, but derivatives of some higher order are discontinuous at the transition point. Synonymous with smooth transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 583

highly oriented pyrolytic graphite

Highly oriented pyrolytic graphite (HOPG) is a pyrolytic graphite with an angular spread of the *c*-axes of the crystallites of less than 1 degree.
Note:
Commercial HOPG is usually produced by stress annealing at approximately $3300\ \mathrm{K}$.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 495

Hildebrand parameter

A parameter measuring the cohesion of a solvent (energy required to create a cavity in the solvent).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1121

hipping

Also contains definition of: hot isostatic pressing

Isostatic pressing process carried out at elevated temperatures.
Notes:

1. The pressurizing fluid used in this process is usually a gas.
2. The temperature is usually in excess of 600 °C.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1823

histones

A class of basic proteins associated with DNA in the chromosomes of eukaryotic cells forming the nucleosome as the basic subunit of chromatin. They contain an unusually large proportion of the basic amino acids arginine and lysine.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

Hofmann rule

"The principal olefin formed in the decomposition of quaternary ammonium hydroxides that contain different primary alkyl groups is always ethylene, if an ethyl group is present." Originally given in this limited form by A. W. Hofmann, the rule has since been extended and modified as follows: "When two or more alkenes can be produced in a β-elimination reaction, the alkene having the smallest number of alkyl groups attached to the double bond carbon atoms will be the predominant product." This orientation described by the Hofmann rule is observed in elimination reactions of quaternary ammonium salts and tertiary sulfonium salts, and in certain other cases.
See also: Zaitsev rule

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1121

hold-back carrier

A carrier used to prevent a particular species from following other species in a chemical or physical operation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

hold-up volume

in chromatography

The volume of eluent required to elute a component, the concentration of which in the stationary phase is negligible compared to that in the mobile phase.

Source:
Orange Book, p. 100

hold-up volume (time), V_{M}, t_{M}

in column chromatography

The volume of the mobile phase (or the corresponding time) required to elute a component the concentration of which in the stationary phase is negligible compared to that in the mobile phase. In other words, this component is not retained at all by the stationary phase. Thus, the hold-up volume (time) is equal to the retention volume (time) of an unretained compound. The hold-up volume (time) includes any volumes contributed by the sample injector, the detector, and connectors.

$$t_{\mathrm{M}} = \frac{V_{\mathrm{M}}}{F_{\mathrm{c}}}$$

In gas chromatography this term is also called the gas hold-up volume (time). The corrected gas hold-up volume ($V^{\mathrm{o}}_{\mathrm{M}}$) is the gas hold-up volume multiplied by the compression (compressibility) correction factor (j):

$$V^{\mathrm{o}}_{\mathrm{M}} = V_{\mathrm{M}}\, j$$

Assuming that the influence of extra column volume on V_{M} is negligible,

$$V^{\mathrm{o}}_{\mathrm{M}} = V_{\mathrm{G}}$$

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 841

hole burning

The photo bleaching of a feature, normally a narrow range, within an inhomogeneous broader absorption or emission band. The holes are produced by the disappearance of resonantly excited molecules as a result of photophysical or photochemical processes. The resulting spectroscopic technique is site-selection spectroscopy.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

hole transfer

Charge migration process in which the majority carriers are positively charged.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

holoenzyme

An active enzyme consisting of the apoenzyme and coenzyme.

Source:
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

Holtsmark broadening [obsolete]

of a spectral line

See: collisional broadening *of a spectral line*

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1463

homo

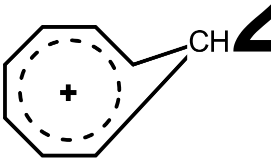
1. An acronym for *H*ighest *O*ccupied *M*olecular *O*rbital (HOMO).
   See: frontier orbitals
2. A prefix (consisting of lower case letters, homo), used to indicate a higher homologue of a compound.

   Source:
   PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1121
3. homo- Affix used to denote a ring expansion by inclusion of a methylene group into a ring-sector.

Source:
Blue Book, p. 500

homoaromatic

Whereas in an aromatic molecule there is continuous overlap of p-orbitals over a cyclic array of atoms, in a homoaromatic molecule there is a formal discontinuity in this overlap resulting from the presence of a single sp^3 hybridized atom at one or several positions within the ring; p-orbital overlap apparently bridges these sp^3 centres, and features associated with aromaticity are manifest in the properties of the compound. Pronounced homoaromaticity is not normally associated with neutral molecules, but mainly with species bearing an electrical charge, e.g. the 'homotropylium' cation, ($C_8H_9{}^+$):



In bis, tris, (etc.) homoaromatic species, two, three, (etc.) single sp^3 centres separately interrupt the π-electron system.
See also: homoconjugation (2)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1121

homochain polymer

A class of polymer in which the main chain is constructed from atoms of a single element. Homochain polymers are named by placing the name or symbol of the element in the main chain immediately before the expression '-chain polymer', e.g. carbon-chain polymer or C-chain polymer; sulfur-chain polymer or S-chain polymer.

Source:
Purple Book, p. 146

homochiral

See: enantiomerically pure (enantiopure)

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

homoconjugation

1. [obsolete] Association between a base and its conjugate acid through a hydrogen bond ($B ... HB^+$ or $AH ... A^-$). Homoassociation is a more appropriate term for this phenomenon.
2. The orbital overlap of two π-systems separated by a non-conjugating group, such as CH_2.
   See also: conjugate acid–base pair, conjugated system, homoaromatic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1121

homocyclic compounds

Cyclic compounds having as ring members atoms of the same element only, e.g. benzene, pentazole, cyclohexasilane.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

homodesmotic reaction

A subclass of isodesmic reactions in which reactants and products contain equal numbers of carbon atoms in corresponding states of hybridization; moreover, there is matching of the carbon-hydrogen bonds in terms of the number of hydrogen atoms joined to the individual carbon atoms. To achieve all this matching, one should significantly extend the number and types of reference molecules. In the aliphatic series of hydrocarbons these are propane, isobutane and neopentanes as well as propene and isobutene; for aromatics—buta-1,3-diene, 2-vinylbutadiene (3-methylidenehexa-1,5-diene) and 2,3-divinylbutadiene (3,4-bismethylidenehexa-1,5-diene). Thus to assess strain energy of cyclopropane and aromatic stabilization of benzene the following homodesmotic reactions are to be respectively analysed.

$\text{c-}(CH_2)_3 + 3\ CH_3\text{–}CH_3 \longrightarrow 3\ CH_3CH_2CH_3$

$\Delta H^0_{\text{exp}} = -26.5\ {}^{\text{kcal}}/_{\text{mol}}\ (110.9\ {}^{\text{kJ}}/_{\text{mol}})$

$C_6H_6 + 3\ CH_2{=}CH_2 \longrightarrow 3\ CH_2{=}CH\text{–}CH{=}CH_2(\textit{trans})$

$\Delta H^0_{\text{calc}}(\text{MP2/6}-31\text{G}^{**}) = 23.9\ {}^{\text{kcal}}/_{\text{mol}}\ (100.0\ {}^{\text{kJ}}/_{\text{mol}})$

Due to closer matching of the hybridization states of the atoms of reactants and products as compared to isodesmic reactions, the homodesmotic reactions give more accurate estimates of the intrinsic strain and the cyclic delocalization. The definition may be extended to molecules with heteroatoms.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1943

homodetic cyclic peptide

A cyclic peptide in which the ring consists solely of amino-acid residues in eupeptide linkage.

Source:
White Book, p. 59

homogeneity

Also contains definition of: heterogeneity *in analytical chemistry*

in analytical chemistry

The degree to which a property or a constituent is uniformly distributed throughout a quantity of material. A material may be homogeneous with respect to one analyte or property but heterogeneous with respect to another. The degree of heterogeneity (the opposite of homogeneity) is the determining factor of sampling error.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1201

homogeneous nucleation

See: embryo, nucleation

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

homogeneous polymer blend

Also contains definition of: miscible polymer blend

Polymer blend that is a single-phase structure.
Notes:

1. Modified from previous definition. The definition proposed here is preferred because it emphasizes the requirement for homogeneity over miscibility.
2. For a polymer blend to be miscible it must obey the thermodynamic criteria of miscibility.
3. Miscibility is sometimes assigned erroneously on the basis that a blend exhibits a single T_g or is optically clear.
4. The miscible system can be thermodynamically stable or metastable.
5. For components of chain structures that would be expected to be miscible, miscibility may not occur if molecular architecture is changed, e.g., by crosslinking.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1817

homoleptic

Transition metal or Main Group compounds having only one type of ligand are said to be homoleptic, e.g. $TaMe_5$.
See also: heteroleptic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1121

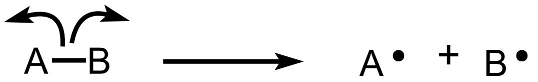
homologous polymer blend

Mixture of two or more fractions of the same polymer, each of which has a different molar-mass distribution.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1988

homolysis (homolytic)

The cleavage of a bond ('homolytic cleavage' or 'homolytic fission') so that each of the molecular fragments between which the bond is broken retains one of the bonding electrons. A unimolecular reaction involving homolysis of a bond (not forming part of a cyclic structure) in a molecular entity containing an even number of (paired) electrons results in the formation of two radicals:



It is the reverse of colligation. Homolysis is also commonly a feature of bimolecular substitution reactions (and of other reactions) involving radicals and molecules.
See also: bond-dissociation energy, heterolysis

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1122

homolytic dissociative adsorption

Relates in the usual sense to the formal nature of the cleavage of a single bond. If the electron pair in the bond of the adsorptive A :B is divided in the course of its dissociative adsorption, the adsorption is homolytic dissociative adsorption.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

homomorphic

Superposable ligands are called homomorphic.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

homopolymer

A polymer derived from one species of (real, implicit or hypothetical) monomer.
Notes:

1. Many polymers are made by the mutual reaction of complementary monomers. These monomers can readily be visualized as reacting to give an 'implicit monomer', the homopolymerization of which would give the actual product, which can be regarded as a homopolymer. Common examples are poly(ethylene terephthalate) and poly(hexamethylene adipamide).
2. Some polymers are obtained by the chemical modification of other polymers such that the structure of the macromolecules that constitute the resulting polymer can be thought of as having

been formed by the homopolymerization of a hypothetical monomer. These polymers can be regarded as homopolymers. Example: poly(vinyl alcohol).

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2300

homopolymerization

Polymerization in which a homopolymer is formed.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2306

homopolysaccharide (homoglycan)

The class name for polysaccharides composed of only one kind of monosaccharide.

Source:
White Book, p. 174

homotopic

Atoms or groups of a molecule which are related by an *n*-fold rotation axis ($n = 2, 3$, etc.) are called homotopic. For example, chiral tartaric acid (C_2 axis), chloroform (C_3 axis) and cyclohexaamylose (α-cyclodextrin, C_6 axis) have respectively two homotopic carboxyl groups, three homotopic chlorine atoms and six homotopic D-glucose residues.
See: prochirality

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

horizontal elution (horizontal development)

in planar chromatography

A mode of operation in which the paper or plate is in a horizontal position and the mobile-phase movement along the plane depends on capillary action.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 829

host

1. A molecular entity that forms complexes with organic or inorganic guests, or a chemical species that can accommodate guests within cavities of its crystal structure. Examples include cryptands and crowns (where there are ion-dipole attractions between heteroatoms and positive ions), hydrogen-bonded molecules that form 'clathrates' (e.g. hydroquinone and water), and host molecules of inclusion compounds (e.g. urea or thiourea). van der Waals forces and hydrophobic interactions bind the guest to the host molecule in clathrates and inclusion compounds.

   Source:
   PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1122
2. (*in biotechnology*) A cell whose metabolism is used for growth and reproduction of a virus, plasmid or other form of foreign DNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

host-vector system

A compatible combination of host (e.g. bacteria) and vector (e.g. plasmid) that allows propagation of DNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

hot atom

An atom in an excited energy state or having kinetic energy above the ambient thermal level, usually as a result of nuclear processes.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

hot cell

A heavily shielded enclosure for highly radioactive materials. It may be used for their handling or processing by remote means or for their storage.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

hot ground state reaction

A hot state reaction of the ground electronic state.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

hot quartz lamp [obsolete]

A term sometimes used to describe a high-pressure mercury lamp. The use of this term is not recommended.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

hot state reaction

A reaction proceeding from an ensemble of molecular entities possessing a higher average vibrational, rotational or translational energy than they would at thermal equilibrium with the surrounding medium.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

hour

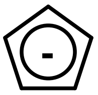
Non-SI unit of time, $\mathrm{h} = 3600\ \mathrm{s}$.

Source:
Green Book, 2nd ed., p. 111
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 976

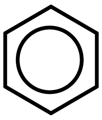
Hückel (4*n* + 2) rule

Monocyclic planar (or almost planar) systems of trigonally (or sometimes digonally) hybridized atoms that contain $(4n + 2)$ π-electrons (where n is a non-negative integer) will exhibit aromatic character. The rule is generally limited to $n = 0$–5. This rule is derived from the Hückel MO calculation on planar monocyclic conjugated hydrocarbons $(\mathrm{CH})_m$ where m is an integer equal to or greater than 3 according to which $(4n + 2)$ π-electrons are contained in a closed-shell system. Examples of systems that obey the Hückel rule include:

cyclopropenyl cation
(= 3, = 0)*mn*



cyclopentadienyl anion
(= 5, = 1)*mn*



benzene
(= 6, = 1)*mn*

Systems containing $4n$ π-electrons (such as cyclobutadiene and the cyclopentadienyl cation) are 'antiaromatic'.
See also: conjugation, Möbius aromaticity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1122

Hückel molecular orbital (HMO) theory

The simplest molecular orbital theory of π-conjugated molecular systems. It uses the following approximations: π-electron approximation; LCAO representation of the π-molecular orbitals; neglect of electron-electron and nuclear-nuclear repulsions (in fact, the assumption that these cancel). The diagonal elements of the effective Hamiltonian, coulombic integrals, and the off-diagonal elements, resonance integrals, (accounted for only directly bonded atoms) are chosen as empirical parameters, all overlap integrals being neglected.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1944

Huggins coefficient, k_{H}

A parameter in the Huggins equation.

Source:
Purple Book, p. 64

Huggins equation

The equation describing the dependence of the reduced viscosity, $\frac{\eta_{\mathrm{i}}}{c}$, on the mass concentration of a polymer, c, for dilute polymer solutions of the form:

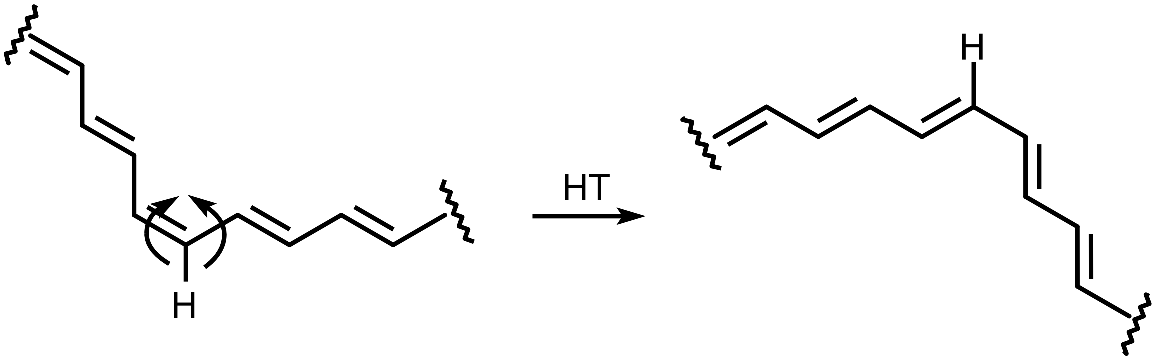
$$\frac{\eta_{\mathrm{i}}}{c} = [\eta] + k_{\mathrm{H}}\,[\eta]^2\,c$$

where k_H is the Huggins coefficient and $[\eta]$ is the intrinsic viscosity.

Source:
Purple Book, p. 63

hula-twist (HT) mechanism

Volume-conserving mechanism of photoisomerization of a double bond in a conjugated system involving simultaneous configurational and conformational isomerization, e.g., the photoinitiated concerted rotation of two adjacent double and single bonds.



Note:
Under unconstrained conditions, the conventional *one-bond-flip* (OBF) process is the dominant process with the hula-twist (HT) being an undetectable higher energy process. It has been proposed that under confined conditions (e.g., a conjugated double bond *chromophore* in a protein cavity or in a solid matrix), the additional viscosity-dependent barriers makes the OBF a less favourable process, allowing the volume-conserving HT to be the dominant process for photoisomerization.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 352

humidity

in atmospheric chemistry

A general term referring to the water content of a gas.
See: relative humidity

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2194

Hund rules

1. Of the different multiplets resulting from different configurations of electrons in degenerate orbitals of an atom those with greatest multiplicity have the lowest energy (multiplicity rule).

2. Among multiplets having the same multiplicity, the lowest-energy one is that with the largest total orbital angular momentum (angular momentum rule) (valid if the total orbital angular momentum is a constant of motion).
3. In configurations containing shells less than half full of electrons, the term having the lowest total angular momentum J lies lowest in energy, whereas in those with shells more than half filled, the term having the largest value of J lies lowest (fine structure rule). Hund rules apply if the 'Russell–Saunders' coupling scheme is valid. Sometimes the first rule is applied with questionable validity to molecules.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2246

Hush model

See: Marcus–Hush relationship

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2247

HWHM (Half Width at Half Maximum)

See: line width

Source:
Green Book, 2nd ed., p. 31

hybrid material

Material composed of an intimate mixture of inorganic components, organic components, or both types of component.
Note:
The components usually interpenetrate on scales of less than $1\ \mu m$.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1811

hybrid orbital

An atomic orbital derived through hybridization of atomic orbitals with different angular momentum quantum numbers located at a given atom.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1944

hybrid polymer

Polymer or polymer network comprised of inorganic and organic components.
Note:
Examples include inorganic–organic polymers and organic–inorganic polymers.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1812

hybridization

1. Linear combination of atomic orbitals on an atom. Hybrid orbitals are often used in organic chemistry to describe the bonding molecules containing tetrahedral (sp^3), trigonal (sp^2) and digonal (sp) atoms.

   Source:
   PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1122
2. The formation of stable duplexes of two DNA and/or RNA (complementary) strands via Watson-Crick base pairing used for locating or identifying nucleotide sequences and to establish the effective transfer of nucleic acid material to a new host.
3. The formation of a novel diploid organism either by sexual processes or by protoplast fusion.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

hybridoma

A hybrid cell line resulting from the fusion of a specific antibody -producing spleen cell (lymphocyte) with a myeloma cell, which has the growth characteristics of the myeloma component and the antibody-secreting characteristics of the lymphocyte, and will multiply to become a source of pure monoclonal antibody.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

hydration

Addition of water or of the elements of water (i.e. H and OH) to a molecular entity. For example, hydration of ethene:

$$\mathrm{H_2C{=}CH_2} \quad + \quad \mathrm{H_2O} \quad \longrightarrow \quad \mathrm{CH_3{-}CH_2{-}OH}$$

The term is also used in a more restricted sense for the process:

$$\text{A (gas)} \longrightarrow \text{A (aqueous soln.)}$$

cf. the use of the term in inorganic/physical chemistry to describe the state of the ions of an electrolyte in aqueous solution.
See also: aquation, solvation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1122

hydrazides

Compounds derived from oxoacids $R_kE(=O)_l(OH)_m$ ($l \neq 0$) by replacing –OH by $-NRNR_2$ (R groups are commonly H), as in carbohydrazides, $RC(=O)NHNH_2$, sulfonohydrazides, $RS(=O)_2NHNH_2$, and phosphonic dihydrazides, $RP(=O)(NHNH_2)_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1340

hydrazidines

Also contains definition of: hydrazide hydrazones

Compounds, $RC(NHNH_2)_2=NNH_2$, derived from carboxylic acids by replacing –OH by $-NHNH_2$ (or *N*-substituted analogues) and =O by $=NNH_2$ (or substituted analogues). A specific hydrazidine is named as a hydrazide hydrazone, e.g. hexanohydrazide hydrazone.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrazines

Hydrazine (diazane), H_2NNH_2, and its hydrocarbyl derivatives. When one or more substituents are acyl groups, the compound is a hydrazide. *N*-Alkylidene derivatives are hydrazones.
See: azines, hydrazo compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrazinylidenes

Synonymous with isodiazenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrazo compounds

Compounds containing the divalent hydrazo group, –NHNH–, such as hydrazoarenes (1,2-diarylhydrazines or 1,2-diaryldiazanes, usually with both aryl groups the same) and their *N*-substituted derivatives ArNRNRAr.
See also: hydrazines

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrazones

Compounds having the structure $R_2C{=}NNR_2$, formally derived from aldehydes or ketones by replacing =O by $=NNH_2$ (or substituted analogues).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrazonic acids

Compounds derived from *oxoacids* $R_kE({=}O)_l(OH)_m$ ($l \neq 0$) by replacing a double-bonded oxygen atom by $=NNR_2$, as in carbohydrazonic acids, $RC(OH){=}NNH_2$ and sulfonohydrazonic acids, $RS({=}O)({=}NNH_2)OH$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrocarbons

Compounds consisting of carbon and hydrogen only.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrocarbyl groups

Univalent groups formed by removing a hydrogen atom from a hydrocarbon, e.g. ethyl, phenyl.
See: heterocyclyl, organoheteryl, organyl groups

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrocarbylene groups

Divalent groups formed by removing two hydrogen atoms from a hydrocarbon, the free valencies of which are not engaged in a double bond, e.g. 1,3-phenylene, $–CH_2CH_2CH_2–$ propane-1,3-diyl, $–CH_2–$ methylene.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrocarbylidene groups

Divalent groups, $R_2C=$, formed by removing two hydrogen atoms from the same carbon atom of a hydrocarbon, the free valencies of which are engaged in a double bond.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrocarbylidyne groups

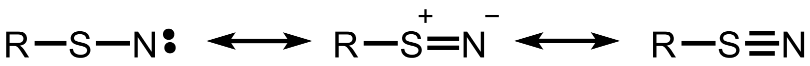
Trivalent groups, $RC\equiv$, formed by removing three hydrogen atoms from the same carbon atom of a hydrocarbon, the free valencies of which are engaged in a triple bond.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrocarbylsulfanyl nitrenes

Synonym: sulfenyl nitrenes

Nitrenes substituted with hydrocarbyl sulfanyl groups,



$$R-S-N\colon \longleftrightarrow R-\overset{+}{S}=\overset{-}{N} \longleftrightarrow R-S\equiv N$$

. Sulfenyl nitrenes is a older synonymous term. E.g. MeSN methylsulfanylnitrene or methylthionitrene. The synonymous term thiazynes (from the third canonical form; confusable with the hetarynes derivable from 1,2- and 1,4-thiazine) is best avoided.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1341

hydrocracking unit

Used in the thermal decomposition of heavy (high molecular weight) hydrocarbons to smaller (low molecular weight) hydrocarbons; high pressures of hydrogen and a special catalyst are employed. Sulfur compounds in the fuel are reduced to H_2S, and the final hydrocarbon product can be obtained relatively sulfur-free.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

hydrodynamic volume

in polymers

The volume of a hydrodynamically equivalent sphere.

Source:
Purple Book, p. 60

hydrodynamically equivalent sphere

in polymers

A hypothetical sphere, impenetrable to the surrounding medium, displaying in a hydrodynamic field the same frictional effect as an actual polymer molecule. The size of a hydrodynamically equivalent sphere may be different for different types of motion of the macromolecule, e.g. for diffusion and for viscous flow.

Source:
Purple Book, p. 60

hydrogel

Gel in which the swelling agent is water.
Notes:

1. The network component of a hydrogel is usually a polymer network.
2. A hydrogel in which the network component is a colloidal network may be referred to as an aquagel.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1807

hydrogen

The general name for the atom H, without regard for its nuclear mass, either for hydrogen in its natural abundance or where it is not desired to distinguish between the isotopes. The systematic name for atomic hydrogen is monohydrogen.
See also: hydron

Source:
PAC, 1988, *60*, 1115 *(Names for hydrogen atoms, ions, and groups, and for reactions involving them (Recommendations 1988))* on page 1116

hydrogen bond

A form of association between an electronegative atom and a hydrogen atom attached to a second, relatively electronegative atom. It is best considered as an electrostatic interaction, heightened by the small size of hydrogen, which permits proximity of the interacting dipoles or charges. Both electronegative atoms are usually (but not necessarily) from the first row of the Periodic Table, i.e. N, O or F. Hydrogen bonds may be inter-molecular or intramolecular. With a few exceptions, usually involving fluorine, the associated energies are less than $20 - 25\ \text{kJ mol}^{-1}$ ($5 - 6\ \text{kcal mol}^{-1}$).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1123

hydrogen bond

in theoretical organic chemistry

A particular type of multicenter (three center - four electron) X–H ...Y in which the central hydrogen atom covalently linked to an electronegative atom X (C, N, O, S..) forms an additional weaker bond with atom Y (N, O, S..) in the direction of its lone electron pair orbital. The energy of hydrogen bonds, which is usually in the range of $3 - 15\ ^{\text{kcal}}/_{\text{mol}}$ ($12 - 65\ ^{\text{kJ}}/_{\text{mol}}$), results from the electrostatic interaction and also from the orbital interaction of the antibonding $\sigma^*(\text{XH})$*MO* of the molecule acting as the hydrogen donor and the non-bonding lone electron pair *MO*n_Y of the hydrogen acceptor molecule.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1945

hydrogen gas electrode

A thin foil of platinum electrolytically coated with a finely divided deposit of platinum or palladium metal, which catalyses the electrode reaction:

$$\text{H}^+ + \text{e} \rightarrow \frac{1}{2}\text{H}_2$$

in solutions saturated with hydrogen gas.

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 540

hydrolases

Enzymes that catalyse the cleavage of C–O, C–N, C–C and other bonds by reactions involving the addition or removal of water.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 156

hydrolysis

Solvolysis by water.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1123

hydrolysis ratio, r_w

Mole ratio of water to alkoxy groups used in sol-gel processing of metal alkoxides.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1823

hydrometeor

in atmospheric chemistry

Any condensed water particle in the atmosphere of sufficient size to be potentially capable of undergoing precipitation (in fogs, clouds, some hazes, raindrops, snowflakes, etc.).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

hydron

Also contains definitions of: hydride, hydro

The general name for the cation H^+; the species H^- is the hydride anion and H is the hydro group. These are general names to be used without regard to the nuclear mass of the hydrogen entity, either for hydrogen in its natural abundance or where it is not desired to distinguish between the isotopes.

Source:
PAC, 1988, *60*, 1115 *(Names for hydrogen atoms, ions, and groups, and for reactions involving them (Recommendations 1988))* on page 1116
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1123
Red Book, p. 103

hydroperoxides

Monosubstitution products of hydrogen peroxide (dioxidane), HOOH, having the skeleton ROOH, in which R is any organyl group. Compounds in which R is acyl are known as peroxy acids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

hydrophilic

'Water loving'. The capacity of a molecular entity or of a substituent to interact with polar solvents, in particular with water, or with other polar groups.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1123

hydrophilicity

Hydrophilicity is the tendency of a molecule to be solvated by water.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1145

hydrophobic interaction

The tendency of hydrocarbons (or of lipophilic hydrocarbon-like groups in solutes) to form intermolecular aggregates in an aqueous medium, and analogous intramolecular interactions. The name arises from the attribution of the phenomenon to the apparent repulsion between water and hydrocarbons. However, the phenomenon ought to be attributed to the effect of the hydrocarbon-like groups on the water-water interaction. The misleading alternative term 'hydrophobic bond' is discouraged.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1123

hydrophobicity

Hydrophobicity is the association of non-polar groups or molecules in an aqueous environment which arises from the tendency of water to exclude non-polar molecules.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1145

hydropolysulfides

Compounds having the structures RS_2H, RS_3H ... RS_nH, in which S_n is a chain of sulfur atoms, and R is hydrocarbyl. Some people exclude hydrodisulfides from the class hydropolysulfides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

hydrosphere

in atmospheric chemistry

The gaseous, liquid and solid water of the earth (oceans, ice caps, lakes, rivers, etc.) as distinguished from the lithosphere and the atmosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

hydrosulfides

Term used in radicofunctional nomenclature of thiols. Hydrosulfides is not commonly used as a class name for thiols.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

hydroxamic acids

Compounds, RC(=O)NHOH, derived from oxoacids $R_kE(=O)_l(OH)_m$ ($l \neq 0$) by replacing –OH by –NHOH, and hydrocarbyl derivatives thereof. Specific examples are preferably named as *N*-hydroxy amides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

hydroximic acids

Compounds derived from oxoacids $R_kE(=O)_l(OH)_m$ ($l \neq 0$) by replacing =O by =NOH (=NOR), as in carbohydroximic acids, RC(OH)=NOH, and sulfonohydroximic acids, RS(=O)(=NOH)OH.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

hydroxylamines

Hydroxylamine, $H_2N–OH$, and its hydrocarbyl derivatives.
See also: hydroxamic acids, oximes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

hygrometer

Instrument used to measure the water vapour content of the atmosphere.
See: capacitance hygrometer, dew point hygrometer, electrical hygrometer, electrolytic hygrometer, frost point hygrometer, mechanical hygrometer, psychrometric hygrometer

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

hygrometry (moisture analysis)

The measurement or indication of the water content of the ambient air or of a sample of gas.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

hyperchromic effect

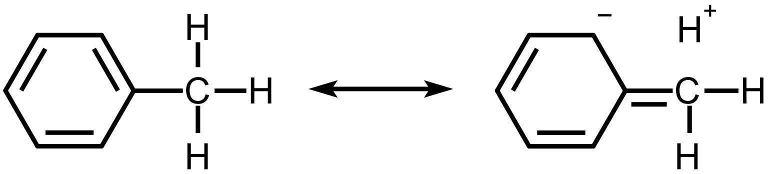
The increase in the intensity of a spectral band due to substituents or interactions with the molecular environment.
See also: auxochrome, hypochromic effect

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2247

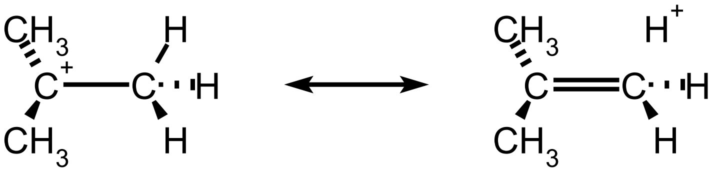
hyperconjugation

Also contains definitions of: heterovalent hyperconjugation, isovalent hyperconjugation, sacrificial hyperconjugation

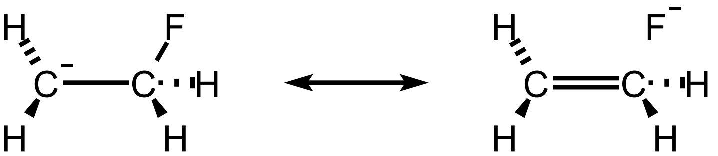
In the formalism that separates bonds into σ and π types, hyperconjugation is the interaction of σ-bonds (e.g. C–H, C–C, etc.) with a π network. This interaction is customarily illustrated by contributing structures, e.g. for toluene (below), sometimes said to be an example of 'heterovalent' or 'sacrificial hyperconjugation', so named because the contributing structure contains one two-electron bond less than the normal Lewis formula for toluene:



At present, there is no evidence for sacrificial hyperconjugation in neutral hydrocarbons. The concept of hyperconjugation is also applied to carbenium ions and radicals, where the interaction is now between σ-bonds and an unfilled or partially filled π- or p-orbital. A contributing structure illustrating this for the *tert*-butyl cation is:



This latter example is sometimes called an example of 'isovalent hyper-conjugation' (the contributing structure containing the same number of two-electron bonds as the normal Lewis formula). Both structures shown on the right hand side are also examples of 'double bond-no-bond resonance'. The interaction between filled π- or p- orbitals and adjacent antibonding σ* orbitals is referred to as 'negative hyperconjugation', as for example in the fluoroethyl anion:



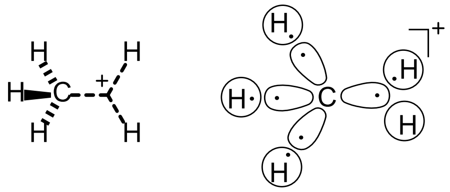
See also: sigma, pi, n-σ*, delocalization

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1123

hypercoordination

A property of main-group atoms in molecular entities to acquire coordination numbers greater than four (which would comply with the Lewis octet rule). Hypercoordination may be associated with hypervalency, but usually is referred to peculiar atomic centres in the electron-deficient species with multicentre σ-bonding, in which the bonding power of a pair of electrons is spread over more than two atoms. An example of a hypercoordinated atom is the five-coordinate carbon atom in the methanium cation, where three C–H bonds may be regarded as normal two center - two electron bonds and the bonding in the remaining CH_2 fragment is governed by the three-centre, two-electron bond.

CH_5^+



A particular case of a hypercoordinated atom is the hydrogen atom included into a hydrogen bond.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1945

hyperfine coupling

The interaction between the spin magnetic moment of an unpaired electron and the nuclear spin magnetic moments resulting in the splitting of the α (spin up) and β (spin down) energy levels in an external magnetic field and, thus, in the multiplet pattern of the ESR spectra of radical-like species and transition metal compounds. Two main contributions to the hyperfine coupling are usually considered, Fermi contact and dipolar interactions. The contact interaction is isotropic and related to the unpaired spin density at the nucleus, $| \psi_\sigma |^2$. The dipolar interaction is anisotropic, and related to r^{-3}, where r is the distance between the atom holding the unpaired electron and the nucleus with non-zero spin.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1945

hyperfine (interaction)

Interaction between the electron spin S and the nuclear spin I.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 353

hyperpolarizability (of *n*th order)

The energy of a molecule in an external electrostatic field can be expanded as

$$E = E^{\mathrm{o}} - \mu_i F_i - \frac{1}{2} \alpha_{ij} F_i F_j - \frac{1}{6} \beta_{ijk} F_i F_j F_k - \frac{1}{24} \gamma_{ijkl} F_i F_j F_k F_l - \ldots$$

where E^{o} is the unperturbed energy, F_i is the component of the field in the i direction, μ_i is the permanent dipole moment, α_{ij} is the polarizability tensor, and β_{ijk} and γ_{ijkl} are the first and second hyperpolarizability tensors, respectively. β is a third order symmetric tensor that measures the second order response of the molecular electric dipole moment to the action of an external electric field and is thus often referred to as dipole hyperpolarizability.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1946

hypervalency

The ability of an atom in a molecular entity to expand its valence shell beyond the limits of the Lewis octet rule. Hypervalent compounds are common for the second and subsequent row elements in groups 15–18 of the periodic table. A description of the hypervalent bonding implies a transfer of the electrons from the central (hypervalent) atom to the nonbonding molecular orbitals which it forms with (usually more electronegative) ligands. A typical example of the hypervalent bond is a linear three-centre, four-electron bond, e.g. that of F_{ap}–P–F_{ap} fragment of PF_5.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1946

hypho-

An affix used in names to designate an open structure, especially a boron skeleton, more closed than a klado structure but more open than an arachno structure.

Source:
Red Book, p. 245

hypo-phase

The denser phase in an extraction system. This term is often used when two non-aqueous phases are present or when the solvent is an aqueous phase.
See also: epi-phase

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2381

hypochromic effect

The opposite of hyperchromic effect (i.e. a decrease in intensity).

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2247

hypsochromic shift

Shift of a spectral band to higher frequency or shorter wavelength upon substitution or change in medium. It is informally referred to as blue shift.
See also: bathochromic shift

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1124
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2247

hysteresis

Also contains definition of: electrode memory

1. Regarding a material quantity or instrument's reading; the dependence of a value on the direction of change from a previous characteristic value. It may be quantified by the difference between the upscale and downscale variation starting from fixed lower and upper measurement points (inversion).

   Source:
   PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196
2. (*in solid-state transitions*) The difference in temperature or pressure for the transition of one phase to another in the forward and reverse directions. It also refers to the corresponding difference in magnetic, electric or stress field in reversing the sense of magnetic, electric or strain polarization in ferromagnetic, ferroelectric or ferroelastic materials.

   Source:
   PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 583
3. (*in electroanalytical chemistry*) Hysteresis (electrode memory) occurs when there is a difference between the emf first observed in a solution containing a concentration of A and a second observation of the emf in the same solution after exposing the electrode to a different concentration of A. The systematic error is generally in the direction of the concentration of the solution in which the electrode was previously immersed. Hysteresis is thought to be a kinetic process. Normal, reversible responses are expected when sufficient time is allowed for the system to return to its initial condition.

See also: electrode memory

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2530

IC

Frequently used acronym for internal conversion.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 354

icosahedro-

An affix used in names to denote twelve atoms bound into a triangular icosahedron.

Source:
Red Book, p. 245
Blue Book, p. 465

icosanoids

Synonym: eicosanoids

Unsaturated C_{20} fatty acids and skeletally related compounds. The spelling icosanoids is preferred over the spelling eicosanoids for consistency with icosanoic acid. Specialists working in this field commonly use eicosanoids, however.
See: prostanoids, leukotrienes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

ICT

Acronym for intramolecular charge transfer.
See also: planar intramolecular charge transfer, , twisted intramolecular charge transfer.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 354

ICT emission

Electronic emission from an ICT state.
See also: intramolecular charge transfer.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 354

ideal, non-linear chromatography

Chromatographic process, where only the curvature of the distribution isotherm determines the shape of the peaks while other peak-broadening processes are neglected.
Note:
The assumption of ideal, non-linear (INL) chromatography is often made in order to facilitate theoretical treatments. It can be justified in cases of efficient columns and distribution isotherms with prominent non-linearity.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1594

ideal adsorbed state

The adsorbed state in a system following Langmuir's isotherm.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 78

ideal chromatography

Chromatographic process, where no peak-broadening effects (such as diffusion, slow mass transfer, *etc.*) operate.
Note:
This is a hypothetical case, implying that the plate number is infinite.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1593

ideal dilute solution

Dilute solution in which the solute may be regarded as obeying Henry's law, so that all the solute activity coefficients may be approximated to 1.

Source:
Physical Chemistry Division, unpublished

See also:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 545

ideal gas

Gas which obeys the equation of state $p\,V = n\,R\,T$ (the ideal gas law; p is the pressure, V the volume, n the amount of molecules, R the gas constant and T the thermodynamic temperature). For an ideal gas the fugacity, f, of each constituent **B** is equal to its partial pressure, p_{B}, $f_{\mathrm{B}} = p_{\mathrm{B}} = x_{\mathrm{B}}\,p$, where x_{B} is the amount fraction of **B**.

Source:
Physical Chemistry Division, unpublished

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

ideal mixture

A mixture of substances **B**, **C**, ... is called an ideal mixture when $a_{\mathrm{B}} = x_{\mathrm{B}}$, $a_{\mathrm{C}} = x_{\mathrm{C}}$, ... or $f_{\mathrm{B}} = 1$, $f_{\mathrm{C}} = 1$ where a_{B} and f_{B} are the relative activity and the activity coefficient, respectively, of a substance **B** in a liquid or solid mixture.

Source:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 543

ideally polarized (electrified) interphase

See: electrified interphase

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

ideally unpolarized (electrified) interphase

See: electrified interphase

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

identity reaction

Synonym: degenerate chemical reaction

A chemical reaction whose products are chemically identical with the reactants, for example the bimolecular self exchange reaction of CH_3I with I^-.
See also: degenerate rearrangement

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1124

illuminance, E, E_{v}

Luminous flux received by a surface divided by the area of that surface.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 976

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

image converter tube

An electron tube that produces on its fluorescent screen an image of the irradiation pattern of its photosensitive input surface. An image converter which produces an image with enhanced radiance is sometimes called an image intensifier.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1758

image dissection tube

A two-dimensional radiation detector in which the electron image produced by a photo-emitting surface, usually a photocathode, is focused in the plane of a defining aperture. Magnetic or electric fields scan this image across the defining aperture.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1756

imaging (photoimaging)

The use of a photosensitive system for the capture, recording and retrieval of information associated with an object using electromagnetic energy.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2247

imbalance

The situation in which reaction parameters that characterize different bond forming or bond breaking processes in the same reaction have developed to different extents as the transition state is approached along some arbitrarily defined reaction coordinate. For example, in the nitroalkane anomaly, the Brønsted β exponent for proton removal is smaller than the Brønsted α for the nitroalkane, because of imbalance between the amount of bond breaking and resonance delocalization in the transition state. Imbalance is common in reactions such as elimination, addition and other complex reactions that involve proton (hydron) transfer.
See also: synchronous, synchronization (principle of nonperfect synchronization)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1124

imbibition

in colloid chemistry

The uptake of a liquid by a gel or porous substance. It may or may not be accompanied by swelling.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 615

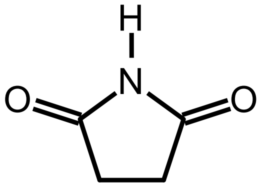
imenes [obsolete]

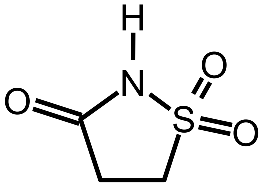
See: nitrenes

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1124

imides

1. Diacyl derivatives of ammonia or primary amines, especially those cyclic compounds derived from diacids, e.g.





2. In additive nomenclature, in which imide is analogous to oxide, the term is used to name compounds of the type R_3Y^+–N^-R (Y = N, P) and R_2Z^+–N^-R (Z = O, S, Se, Te), which are the products of formal attachment of an RN= group to N, P, O, S, Se, Te. E.g. amine imides, azomethine imides.
3. Salts having the anion RN^{2-}.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

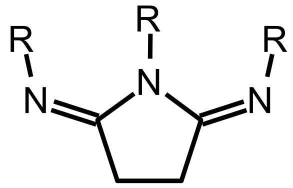
imidic acids

Compounds derived from oxoacids $R_kE(=O)_l(OH)_m$ ($l \neq 0$) by replacing =O by =NR; thus tautomers of amides. In organic chemistry an unspecified imidic acid is generally a carboximidic acid, RC(=NR)(OH) . E.g. $RS(=NH)_2(OH)$ a sulfonodiimidic acid.
See: imino acids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

imidines

Analogues of cyclic acid anhydrides in which =O has been replaced by =NR and –O– by –NR–.



See: diamidides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1342

imidogens [obsolete]

A non-IUPAC term for nitrenes used in the Chemical Abstracts Service index nomenclature.

Source:
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

imidonium ions [obsolete]

A term, which is not recommended, for nitrenium ions.

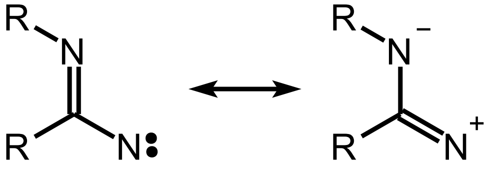
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

imidoyl carbenes

Carbenes having the structure RC(=NR)C:–R. Imidoyl is a shortened but imprecise term for carboximidoyl, RC(=NH)– .

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

imidoyl nitrenes

Nitrenes having the structure  .

See: imidoyl carbenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

imin [obsolete]

See: nitrenes

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1124

imine radical [obsolete]

See: nitrenes

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1124

imines

1. Compounds having the structure $RN{=}CR_2$ (R = H, hydrocarbyl). Thus analogues of aldehydes or ketones, having NR doubly bonded to carbon; aldimines have the structure $RCH{=}NR$, ketimines have the structure $R'_2C{=}NR$ ($R' \neq H$). Imines include azomethines and Schiff bases. Imine is used as a suffix in systematic nomenclature to denote the C=NH group excluding the carbon atom.
2. [obsolete] An obsolete term for azacycloalkanes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

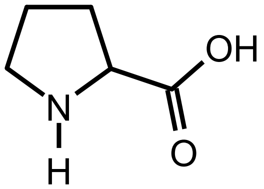
iminium compounds

Salts in which the cation has the structure $R_2C{=}N^+R_2$. Thus *N*-hydronated imines and their *N*-substituted derivatives. The synonymous terms imonium compounds and immonium compounds are irregularly formed and should not be used.
See: quaternary ammonium compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

imino acids

1. An obsolete term, which should not be used, for imidic acids.
2. Any carboxylic acid having an imino substituent, HN=, replacing two hydrogens. A shortened form of imino carboxylic acid.
3. Obsolescent term for azaalkanoic acids and azacycloalkane-2-carboxylic acids, e.g. proline:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

imino carbenes

This term systematically means carbenes bearing an imino or *N*-substituted imino group, RN=, somewhere in the molecule. E.g. R–C:–CH_2C(=NR)R. It is listed here in order to warn against its misuse for alkylideneamino carbenes.
See: carbenes, nitrile ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

iminooxy (iminoxy) radicals [obsolete]

This term has improperly been used for alkylideneaminoxyl radicals, also called iminoxyl radicals R_2C=N–$O^{\cdot}$. Its use is strongly discouraged.
See: aminoxyl radicals, iminyl radicals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

iminoxyl radicals

Synonymous with alkylideneaminoxyl radicals. The term can be regarded as a contraction of iminyloxyl radicals.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

iminyl carbenes

See: nitrile ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

iminyl radicals

Radicals having the structure $R_2C{=}N^{\cdot}$. A contraction of alkaniminyl radicals, e.g. $CH_3{-}CH{=}N^{\cdot}$ ethaniminyl. A synonymous term is alkylideneaminyl radicals.
See: aminyl radicals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1343

iminylium ions

Cations having the structure $R_2C{=}N^+$. A contraction of alkaniminylium ions. Alkylideneaminylium ions is a synonymous term. A subclass of nitrenium ions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

immersional wetting

A process in which a solid or liquid, β, is covered with a liquid, α, both of which were initially in contact with a gas or liquid, δ, without changing the area of the $\alpha\delta$-interface.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 598

immiscibility

Inability of a mixture to form a single phase.
Notes:

1. Immiscibility may be limited to certain ranges of temperature, pressure, and composition.
2. Immiscibility depends on the chemical structures, molar-mass distributions, and molecular architectures of the components.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1990

immiscible polymer blend

Also contains definition of: heterogeneous polymer blend

Polymer blend that exhibits immiscibility.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1990

immission dose

in atmospheric chemistry

The integral of the immission flow into the receptor over the exposure period.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

immission flux

in atmospheric chemistry

The immission rate divided by the unit surface area of the receptor.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

immission

in atmospheric chemistry

A Germanic term, pronounced in English, 'eye-mission'; the transfer of pollutants from the atmosphere to a 'receptor'; for example, pollutants retained by the lungs. It does not have the same meaning as ground level concentration, but is the opposite in meaning to emission. This term has not been used commonly in the English language.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

immission rate

in atmospheric chemistry

The mass (or other physical quantity) of pollutant transferring per unit time into a receptor.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

immobile adsorption

A situation in which the freedom of molecules of adsorbate to move about the surface is limited. Adsorption is immobile when $k\,T$ is small compared to ΔE, the energy barrier separating adjacent sites. The adsorbate has little chance of migrating to neighbouring sites and such adsorption is necessarily localized.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

immobilization

in biotechnology

The technique used for the physical or chemical fixation of cells, organelles, enzymes, or other proteins (e.g. monoclonal antibodies) onto a solid support, into a solid matrix or retained by a membrane, in order to increase their stability and make possible their repeated or continued use. The principle is also used for affinity chromatography.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 157

immobilized enzyme

A soluble enzyme bound to an insoluble organic or inorganic matrix, or encapsulated within a membrane in order to increase its stability and make possible its repeated or continued use.

Source:
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

immobilized phase

in chromatography

A stationary phase in which is immobilized on the support particles, or on the inner wall of the column tubing e.g. by *in situ* polymerization (cross-linking) after coating.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 823

immune response

Selective reaction of the body to substances that are foreign to it, or that the immune system identifies as foreign, shown by the production of antibodies and antibody-bearing cells or by a cell-mediated hypersensitivity reaction.

See also: antibody

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2058

immunization

The administration of an antigen to an animal in order to stimulate the production of antibodies by that organism. Also, the administration of antigens, antibodies or lymphocytes to an animal to generate the corresponding active, passive or adaptive immunity.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 157

immunoassay

A ligand-binding assay that uses a specific antigen or antibody, capable of binding to the analyte, to identify and quantify substances. The antibody can be linked to a radiosotope (radioimmunoassay, RIA), or to an enzyme which catalyses an easily monitored reaction (enzyme-linked immunosorbent assay, ELISA), or to a highly fluorescent compound by which the location of an antigen can be visualized (immunofluorescene).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 157
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

immunochemistry

Study of biochemical and molecular aspects of immunology, especially the nature of antibodies, antigens and their interactions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2058

immunogen

A substance that elicits a cellular immune response and/or antibody production (cf. antigen).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 157

immunoglobulin (Ig)

A protein of the globulin-type found in serum or other body fluids that possesses antibody activity. An individual Ig molecule is built up from two light (L) and two heavy (H) polypeptide chains linked together by disulfide bonds. Igs are divided into five classes based on antigenic and structural differences in the H chains.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 157

immunoradiometric assay

An assay based on the reversible and non-covalent binding of an antigen by a specific antibody labelled with a radioactive nuclide as a tracer.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

immunosuppression

Reduction in the functional capacity of the immune response; may be due to:

1. Inhibition of the normal response of the immune system to an antigen.
2. Prevention, by chemical or biological means, of the production of an antibody to an antigen by inhibition of the processes of transcription, translation or formation of tertiary structure.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2058

impact parameter, b

In simple hard sphere collision theory the distance of closest approach that would result for two particles in a collision if the particle trajectories were undeflected by the collision.

Source:
Green Book, 2nd ed., p. 56
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 168

impact-modified polymer

Polymeric material whose impact resistance and toughness have been increased by the incorporation of phase microdomains of a rubbery material.
Note:

An example is the incorporation of soft polybutadiene domains into glassy polystyrene to produce high-impact polystyrene.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 899

impaction

A forcible contact of particles of matter with a surface.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

impedance, Z

Complex representation of potential difference divided by the complex representation of the current.

Source:
Green Book, 2nd ed., p. 15
ISO 31-4: 1992
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 976

impingement

Equivalent to impaction; often refers to impaction on a liquid surface.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

impinger

A sampling instrument employing impingement for the collection of particulate matter. Common types are:

1. the midget impinger employing impingement in $1\ \mathrm{cm}^3$-$10\ \mathrm{cm}^3$ water,
2. the standard impinger employing impingement in $75\ \mathrm{cm}^3$ water and
3. dry impingers.

Impingers are also suitable for sampling certain gases and vapours.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

imprecision

in analysis

Variation of the result in a set of replicate measurements. This can be expressed, e.g. as the standard deviation or coefficient of variation (relative standard deviation). This term may have a more general meaning, e.g. if the replicates constitute a batch or involve different instruments, laboratories and analyst.
See: precision

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1706

impregnation

in chromatography

The modification of the separation properties of the chromatographic bed used in planar chromatography by appropriate additives.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 830

impregnation

in polymer chemistry

Penetration of monomeric, oligomeric, or polymeric liquids into an assembly of fibres.
Notes:

1. The term as defined here is specific to polymer science. An alternative definition of 'impregnation' applies in some other fields of chemistry.
2. Impregnation is usually carried out on a woven fabric or a yarn.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1991

improved canonical variational transition-state theory (ICVTST)

A modification of canonical variational transition-state theory in which, for energies below the threshold energy, the position of the dividing surface is taken to be that of the microcanonical threshold energy. This forces the contributions to rate constants to be zero below the threshold energy. A compromise dividing surface is then chosen so as to minimize the contributions to the rate constant made by reactants having higher energies.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 168

in situ micro-X-ray diffraction (Kossel-technique)

Any technique which utilizes the diffraction of X-rays generated in a microstructural domain of a solid under bombardment with a finely focused electron beam, thus providing an X-ray diffraction pattern of this microstructural domain. The pattern can be recorded with a film either on the reflection or transmission side of the specimen (in the latter case the crystalline sample has to be a thin film or a small particle).

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2025

in situ microanalysis

Term used for direct analytical investigation of the microstructural domains of a solid by focused beams of particles and radiation. Analytical characterization includes obtaining information about type, quantity and distribution of the elements, their state of chemical bonding, morphology and crystalline (geometric) and electronic structure of the individual phases. The combination of this information serves as a basis for the property-relevant characterization of solids.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2024

in vitro

In glass, referring to a study in the laboratory usually involving isolated organ, tissue, cell, or biochemical systems.
See also: in vivo

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2061

in vivo

In the living body, referring to a study performed on a living organism.
See also: in vitro

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2061

in-laboratory processing

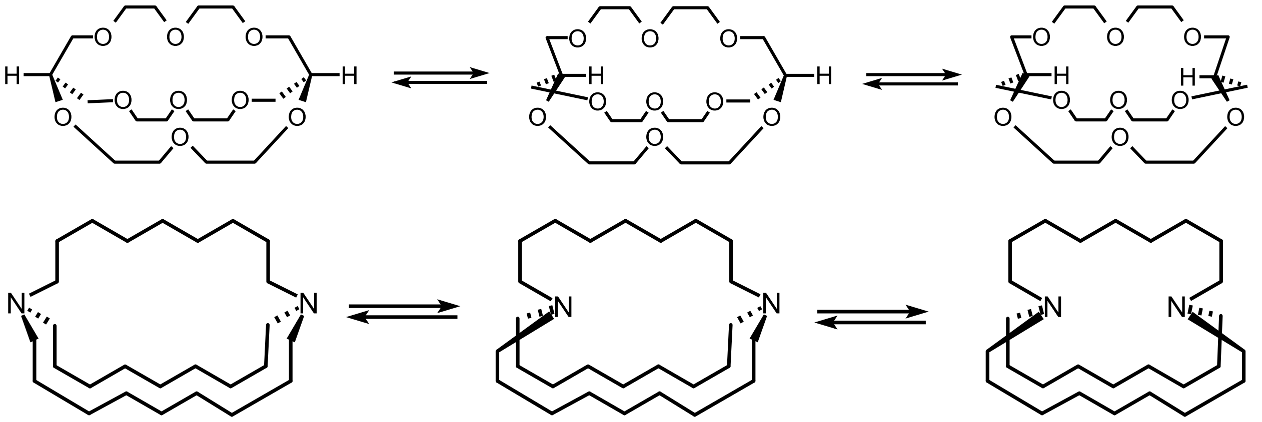
in analytical chemistry

The selection, removal and preparation of the test (or analytical) portions from the laboratory sample. The processing may include a reduction in the size of the unit(s) (division) and particle size (reduction), as well as mixing to achieve homogeneity.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1204

in-out isomerism

Isomerism found in bicyclic systems having long enough bridges to allow the bridgehead exocyclic bond or lone pair of electrons to point either inside the structure or outside.



Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

in-situ composite formation

Process for preparing a polymer composite by

1. forming the filler or reinforcement in an existing polymer or
2. polymerizing monomers in the presence of dispersed filler.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1823

inaccuracy

in analysis

A quantitative term to describe the (lack of) accuracy of a chemical measurement process; comprises the imprecision and the bias. Inaccuracy must be viewed as a two-component quantity (vector); imprecision and bias should never be combined to give a scalar measure for chemical measurement

process inaccuracy. (One or the other component may, however, be negligible under certain circumstances.) Inaccuracy should not be confused with uncertainty. Inaccuracy (imprecision, bias) is characteristic of the measurement process, whereas error and uncertainty are characteristics of a result. (The latter characteristic, of course, derives from the imprecision and bounds for bias of the chemical measurement process.)
Note:
The resultant bias and imprecision for the overall measurement process generally arise from several individual components, some of which act multiplicatively (e.g. sensitivity), and some of which act additively (e.g. the blank).

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1706
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663

inch

Non-SI unit of length, $\mathrm{in} = 0.0254\ \mathrm{m}$.

Source:
Green Book, 2nd ed., p. 110

incidence

in medicinal chemistry

Number of occurrences of illness commencing, or of persons falling ill, during a given period in a specific population: usually expressed as a rate.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1054

incinerator

Equipment in which solid, liquid or gaseous combustible wastes are ignited and burned. Types include flue-fed and multiple-chamber incinerators with several stages of combustion.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

inclusion compound (inclusion complex)

A complex in which one component (the host) forms a cavity or, in the case of a crystal, a crystal lattice containing spaces in the shape of long tunnels or channels in which molecular entities of a second chemical species (the guest) are located. There is no covalent bonding between guest and host, the attraction being generally due to van der Waals forces. If the spaces in the host lattice are enclosed

on all sides so that the guest species is 'trapped' as in a cage, such compounds are known as clathrates or 'cage compounds'.
See also: crown, cryptand, cryptate, intercalation compounds

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1124
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

incoherent radiation

Not having the properties of coherent radiation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2247

increment (for bulk materials and large units)

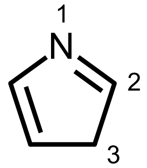
An individual portion of material collected by a single operation of a sampling device. Increments may be reduced individually or tested either (a) individually or (b) combined with other increments with the resulting composite reduced in size and tested as a single unit. Increments are created by the sampling operation and are usually taken from parts of a lot separated in time or space. Increments of a bulk population correspond to units of a packaged population.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1205

indicated hydrogen

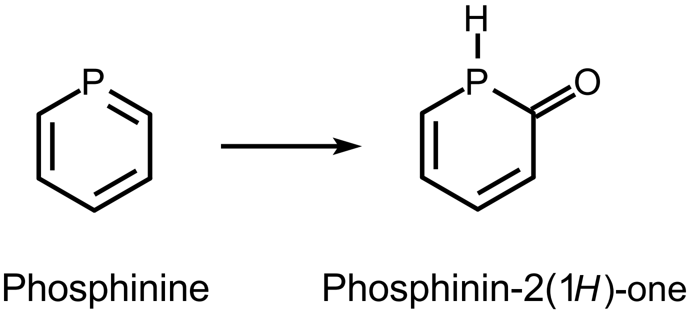
Also contains definition of: added hydrogen

Under certain circumstances it is necessary to indicate in the name of a ring, or ring system, containing the maximum number of non-cumulative double bonds, one or more positions where no multiple bond is attached. This is done by specifying the presence of an 'extra' hydrogen atom at such positions by citation of the appropriate numbered locant followed by an italicized capital *H*. Example:



3*H*-Pyrrole

A second type of indicated hydrogen (sometimes referred to as 'added hydrogen') describes hydrogen atoms added to a specific structure as a consequence of the addition of a suffix or a prefix describing a structural modification. This type of indicated hydrogen is normally cited in parentheses after the locant of the additional feature. Example:



Source:
Blue Book (Guide), p. 34

indicator electrode

An electrode that serves as a transducer responding to the excitation signal (if any) and to the composition of the solution being investigated, but that does not affect an appreciable change of bulk composition within the ordinary duration of a measurement.

Source:
Orange Book, p. 59

indicator (visual)

See: acid-base indicator, adsorption indicator, mixed indicator, colour indicator

Source:
Orange Book, p. 48

indifferent absorbing ion

An ion which absorbs through Coulomb forces only and which is hence only repelled by surfaces of like sign, attracted by surfaces of opposite sign, and is not absorbed on an uncharged surface.
See also: specifically absorbing ion

Source:
PAC, 1991, *63*, 895 *(Nomenclature, symbols, definitions and measurements for electrified interfaces in aqueous dispersions of solids (Recommendations 1991))* on page 899

indifferent electrolyte

Synonymous with supporting electrolyte.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1501

indirect amplification

A type of amplification reaction where the constituent required is associated with some other constituent which is then amplified and measured.

Source:
PAC, 1982, *54*, 2553 *(Recommendations on use of the term amplification reactions)* on page 2555

indirect reaction

A chemical process in which the reactive complex has a lifetime that is longer than its period of rotation is called an indirect reaction (in contrast to a direct reaction). In a molecular-beam experiment the products of such reactions are scattered at random with reference to the centre of mass of the system. Indirect reactions are also called complex-mode reactions (They are sometimes called complex reactions, but this usage is not recommended in view of the danger of confusion with composite reactions, which occur in more than one step).

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 168

individual gauge for localized orbitals (IGLO)

A method of calculation of nuclear shieldings, in which localized molecular orbitals associated with inner shell, bonding orbitals, and lone pairs have unique origins for the calculation of diamagnetic and paramagnetic terms. With this method, satisfactory estimates of NMR chemical shifts for elements in the first and second rows can be achieved in *ab initio* calculations with basis sets of moderate size provided sufficiently accurate molecular geometries are used.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1946

individual perception threshold
Acronym: IPT

in atmospheric chemistry

A term used in odour testing which signifies the lowest concentration of a particular species at which a subject indicates both an initial positive and repeated response.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

induced radioactivity

Radioactivity induced by irradiation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1544

induced reaction

Also contains definition of: inductor

A reaction which occurs or is accelerated only if another reaction is simultaneously occurring in the same system. The substance, which causes an induced reaction, is termed inductor. The inductor, unlike the catalyst, is used up irreversibly during the process.

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2295

inducer

in enzyme catalysis

A small molecule that triggers gene transcription by binding to a regulator protein (cf. enzyme induction). It acts by combining with the corresponding repressor protein to bring about an allosteric change so that the repressor is made incapable of combining with the operator of the system.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 157

induction

in enzyme catalysis

1. An increase in the rate of synthesis of an (inducible) enzyme in response to the action of an inducer or environmental conditions. An inducer is often the substrate of the inducible enzyme or a structurally similar substance (gratuitous inducer) that is not metabolized.
2. The experimental elicitation of lytic growth by a prophage from lysogenic bacteria.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 157
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

induction period

The initial slow phase of a chemical reaction which later accelerates. Induction periods are often observed with radical reactions, but they may also occur in other systems (for example before steady-state concentration of the reactants is reached).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1124
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 169

inductive effect

In strict definition, an experimentally observable effect (on rates of reaction, etc.) of the transmission of charge through a chain of atoms by electrostatic induction. A theoretical distinction may be made between the field effect, and the inductive effect as models for the Coulomb interaction between a given site within a molecular entity and a remote unipole or dipole within the same entity. The experimental distinction between the two effects has proved difficult, except for molecules of peculiar geometry, which may exhibit 'reversed field effects'. Ordinarily the inductive effect and the field effect are influenced in the same direction by structural changes in the molecule and the distinction between them is not clear. This situation has led many authors to include the field effect in the term 'inductive effect'. Thus the separation of values into inductive and resonance components does not imply the exclusive operation of a through-bonds route for the transmission of the non-conjugative part of the substituent effect. To indicate the all-inclusive use of the term inductive, the phrase 'so-called inductive effect' is sometimes used. Certain modern theoretical approaches suggest that the 'so-called inductive effect' reflects a field effect rather than through-bonds transmission.
See also: mesomeric effect, polar effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1124

inductomeric effect

A molecular polarizability effect occurring by the inductive mechanism of electron displacement. The consideration of such an effect and the descriptive term have been regarded as obsolescent or even obsolete, but in recent years theoretical approaches have reintroduced substituent polarizability as a factor governing reactivity, etc. and its parametrization has been proposed.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1125

inelastic scattering

If in a molecular collision there is transfer of energy among degrees of freedom, but no chemical reaction occurs, there is said to be inelastic scattering.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 169

inert

Stable and unreactive under specified conditions.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1125

inert gas

A non-reactive gas under particular conditions. For example, nitrogen at ordinary temperatures and the noble gases (helium, argon, krypton, xenon and radon) are unreactive toward most species.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

inertial defect

Difference of principal moments of inertia $\Delta = I_C - I_A - I_B$. For planar molecules it is close to zero and for non-planar molecules it is negative.

Source:
Green Book, 2nd ed., p. 23

inertial separator

Any dry type collector which utilizes the relatively greater inertia of particles to effect their removal from a gas stream; e.g. cyclonic and impingement separators, gravity settling chambers and high-velocity gas reversal chambers.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

infinite source thickness

For a specified radiation, the minimum thickness of a flat preparation of a radioactive material where the intensity of the specified radiation at the surface does not increase when the thickness is increased by adding more of similar radioactive material.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1544

information theory

As applied in reaction dynamics, information theory analyses the deviations of experimentally-determined energy distributions from predictions made on the basis of equal *a priori* probabilities for all possible outcomes.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 169

infrared

Region of the electromagnetic spectrum extending from 780 nm to about 20 000 nm.
According to the CIE, the range between 780 nm and 1 mm is subdivided into:
IR-A 780–1400 nm
IR-B 1.4–3 μm
IR-C 3 μm–1 mm
Note:
This is the wavelength region in which absorption by a molecular entity causes excitation of its vibrational, rotational, and bending modes.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 354

inherent viscosity

Synonym: logarithmic viscosity number

of a polymer

The ratio of the natural logarithm of the relative viscosity, η_{r}, to the mass concentration of the polymer, c, i.e.

$$\eta_{\mathrm{inh}} \equiv \eta_{\mathrm{ln}} = \frac{\ln \eta_{\mathrm{r}}}{c}$$

The quantity η_{ln}, with which the inherent viscosity is synonymous, is the logarithmic viscosity number.
Notes:

1. The unit must be specified; $\mathrm{cm}^3\ \mathrm{g}^{-1}$ is recommended.
2. These quantities are neither viscosities nor pure numbers. The terms are to be looked on as traditional names. Any replacement by consistent terminology would produce unnecessary confusion in the polymer literature.

Source:
Purple Book, p. 63

inhibition

Also contains definition of: degree of inhibition

The decrease in rate of reaction brought about by the addition of a substance inhibitor), by virtue of its effect on the concentration of a reactant, catalyst or reaction intermediate. For example, molecular oxygen and *p*-benzoquinone can react as 'inhibitors' in many reactions involving radicals as intermediates by virtue of their ability to act as scavengers toward these radicals. If the rate of a reaction in the absence of inhibitor is v_0 and that in the presence of a certain amount of inhibitor is v, the degree of inhibition (i) is given by:

$$i = \frac{v_0 - v}{v_0}$$

See also: mechanism based inhibition

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1125
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 169

See also:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 157
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2295

inhibitor

Also contains definition of: enzyme inhibitor

A substance that diminishes the rate of a chemical reaction; the process is called inhibition. Inhibitors are sometimes called negative catalysts, but since the action of an inhibitor is fundamentally different from that of a catalyst, this terminology is discouraged. In contrast to a catalyst, an inhibitor may be consumed during the course of a reaction. In enzyme-catalysed reactions an inhibitor frequently acts by binding to the enzyme, in which case it may be called an enzyme inhibitor.
See also: effector

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2295

See also:
PAC, 1991, *63*, 1227 *(Manual on catalyst characterization (Recommendations 1991))* on page 1244

inhibitory concentration (IC)

Concentration of a substance that causes a defined inhibition of a given system: IC_{50} is the median concentration that causes 50% inhibition.
See also: lethal concentration

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2060

inhibitory dose (ID)

Dose of a substance that causes a defined inhibition of a given system: ID_{50} is the median dose that causes 50% inhibition.
See also: lethal dose

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2060

inhomogeneity error

in spectrochemical analysis

An error due to inhomogenous distribution of absorbing species in the analytical sample. It may be observed by probing the sample volume with an incident beam of radiation of reduced cross-section.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1456

initial (final) state correlations

These are correlations between the states of the products of a reaction and the initial states of the reactants. The correlations may relate to energy levels, quantum numbers, and symmetries.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 169

initial rate method

A mode of measurement in a kinetic method of analysis, in which the initial reaction rate is determined (usually by the slope method) and utilized for the measurement of concentration.

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2296

initiation

A reaction or process generating free radicals (or some other reactive reaction intermediates) which then induce a chain reaction. For example, in the chlorination of alkanes by a radical mechanism the initiation step is the dissociation of molecular chlorine.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1125
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 169

initiator

A substance introduced into a reaction system in order to bring about an initiation reaction.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 170
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 74

injection temperature

in chromatography

The temperature at the point of injection.

Source:
Orange Book, p. 100

inner electric potential, ϕ

Quantity the gradient of which is equal to the negative of the electric field strength within the phase concerned. It can be calculated from the model of the phase. It is sometimes called the Galvani potential.

Source:
Green Book, 2nd ed., p. 59

inner filter effect

1. In an emission experiment, an apparent decrease in emission quantum yield and/or distortion of bandshape as a result of reabsorption of emitted radiation.
2. During a light irradiation experiment, absorption of incident radiation by a species other than the intended primary absorber.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2247

inner Helmholtz plane (IHP)

The locus of the electrical centres of specifically adsorbed ions.
See also: outer Helmholtz plane

Source:
PAC, 1991, *63*, 895 *(Nomenclature, symbols, definitions and measurements for electrified interfaces in aqueous dispersions of solids (Recommendations 1991))* on page 899
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 448

inner layer (compact layer)

in electrochemistry

The region between the outer Helmholtz plane and the interface.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1261

inner orbital X-ray emission spectra

X-ray spectral lines generated by the transition of electrons between 'inner orbitals'. The term 'inner orbital' serves to designate the sharp, not degenerate electronic levels of atoms in a solid and therefore is a general term for all orbitals except the valence band.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2026

inner-sphere electron transfer

Historically an electron transfer between two metal centres sharing a ligand or atom in their respective coordination shells. The definition has more recently been extended to any situation in which the interaction between the donor and acceptor centres in the transition state is significant ($> 20\ \mathrm{kJ\ mol^{-1}}$).
See also: outer-sphere electron transfer

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1125
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2247

inoculation

The introduction of a small sample of organisms (microbial, plant or animal cells) into a culture medium to act as a seed for the production of large numbers of the same organism by growth and propagation.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

inorganic polymer

Polymer or polymer network with a skeletal structure that does not include carbon atoms.
Note:
Examples include polyphosphazenes, polysilicates, polysiloxanes, polysilanes, polysilazanes, polygermanes, polysulfides, *etc*.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1812

inorganic–organic polymer

Acronym: IOP

Polymer or polymer network with a skeletal structure comprising inorganic and organic units.
Note:
Examples include poly(carbasilane)s, poly(phenylenesilanediyl)s, poly(phenylenesulfide)s, *etc*.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1812

inositols

Cyclohexane-1,2,3,4,5,6-hexols.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

See also:
White Book, p. 151

input rate

in analysis

The number of samples that are processed by the instrument divided by time of operation. It should be stated if the residence time is included or not.

See: residence time

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663

insert

in biotechnology

A sequence of foreign DNA introduced into a restriction site (insertion site, cloning site) of a vector DNA.

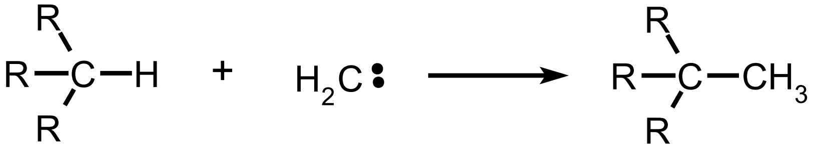
Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

insertion

1. A chemical reaction or transformation of the general type:

$$X{-}Z + Y \longrightarrow X{-}Y{-}Z$$

   in which the connecting atom or group Y replaces the bond joining the parts X and Z of the reactant XZ. An example is the carbene insertion reaction:



   The reverse of an insertion is called an extrusion.
   See also: α-addition

   Source:
   PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1125
2. A general term given to a reaction involving the transfer of a guest atom, ion or molecule into a host crystal lattice.
   See: intercalation reaction, topochemical reaction, topotactic reaction

   Source:
   PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 583

instability of Hartree–Fock solution

Existence of additional solutions to the equations of the Hartree–Fock method occurring usually in the case when potential energy surfaces of different electronic states are drawn close together. Within the spin-restricted Hartree–Fock method (RHF), singlet and triplet instabilities are distinguished. The former involves the existence of another solution with lower energy and the electron distribution of lower symmetry. It may be regarded as an indication that the initially assumed molecular shape needs correction. The triplet instability involves rejection of the condition of double occupancy of molecular orbitals and thus transition to the spin-unrestricted Hartree–Fock method (UHF). The triplet instability is a necessary, but insufficient, condition for the conclusion as to the biradical character of the ground state of a given system.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1946

instability (with reference to instrumentation)

A change which takes place in an instrument reading over a stated period of unattended operation for a given value of the air quality characteristic. It can be characterized by the variation with time of its mean, specifying the drift and by the dispersion. Span instability is the change which takes place in instrument span over a stated period of unattended operation. Zero instability is the change in instrument reading in response to a zero sample over a stated period of unattended operation.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2197

instantaneous current

At a dropping electrode, the total current that flows at the instant when a time t has elapsed since the fall of the preceding drop. At any other electrode, the total current that flows at the instant when a time t has elapsed since the beginning of an electrolysis. The instantaneous current is usually time-dependent and may have the character of an adsorption, catalytic, diffusion, double-layer, or kinetic current, and may include a migration current. A plot of the dependence of instantaneous current on time is commonly called an 'i-t curve'.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1496

instantaneous rate of flow

in polarography

The rate of increase of the mass of a drop at a particular instant t seconds after it has begun to form.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1504

instantaneous (spot) sampling

in atmospheric chemistry

Obtaining a sample of the atmosphere in a period which is short compared with the duration of the sampling exercise. Such samples are often called 'grab' samples, a term not recommended. These are useful for the analysis of hydrocarbons and other complicated mixtures of trace gases which are relatively stable in a stainless steel canister or tank and can be transported back to the laboratory for chromatographic or other analysis which cannot be done satisfactorily in the field.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2197

instrumental activation analysis

A kind of activation analysis in which element specificity is obtained by using appropriate irradiation conditions, radiation measurement techniques and mathematical techniques for the interpretation of the measurement results.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515

instrumental dependability

This relates to the frequency of failures which interrupt the operation of an instrument. It can be quantified, e.g. by the infrequency of breakdowns or by the availability of the instrument for use when required.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663

instrumental indication (for a precision balance)

The observed deflection or rest point multiplied by the value of the division for the load in question.

Source:
Orange Book, p. 36

integral capacitance

of an electrode

Integral capacitance (per unit area of electrode) is given by

$$K = \frac{Q}{E - E_{Q=0}}$$

where Q is the electric charge (per unit area of electrode), E is the potential of the electrode with respect to a reference electrode, and $E_{Q=0}$ is the potential at the point of zero charge.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 509

integral detector

in chromatography

A device which measures the accumulated quantity of sample component(s) reaching the detector.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 849

integrating sphere

A hollow sphere having a highly reflecting inside surface used as a device to collect, with very high efficiency, light scattered or emitted from a sample contained in it or located outside and near one of the ports. Small ports allow the entrance of light and access to a detector.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2248

intended crossing

of potential-energy surfaces

Synonymous with avoided crossing. The term 'intended' should not be used in this context since it is an anthropomorphic term.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2248

intensity

1. The traditional term for photon flux, fluence rate, irradiance or radiant power (radiant flux). In terms of an object exposed to radiation, the term should now be used only for qualitative descriptions.

   Source:
   PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2248

   See also:
   Orange Book, p. 228
   Green Book, 2nd ed., p. 31

PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2197

2. The magnitude of a particular feature in a spectrum.

   Source:
   PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2248

intensity (relative to base peak)

in mass spectrometry

The ratio of intensity of a separated ion beam to the intensity of the separated ion beam which has the greatest intensity. This ratio is generally equated to the normalized ratio of the heights of the respective peaks in the mass spectrum, with the height of the base peak being taken as 100.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1554
Orange Book, p. 206

intensive quantity

Physical quantity whose magnitude is independent of the extent of the system.

Source:
Green Book, 2nd ed., p. 7

interaction distance

The farthest distance of approach of two particles at which it is discernible that they will not pass at the impact parameter.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

intercalation compounds

Compounds resulting from reversible inclusion, without covalent bonding, of one kind of molecule in a solid matrix of another compound, which has a laminar structure. The host compound, a solid, may be macromolecular, crystalline or amorphous.
See also: inclusion compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

intercalation

in polymer chemistry

Process by which a substance becomes transferred into pre-existing spaces of molecular dimensions in a second substance.
Note:
The term as defined here is specific to polymer science. An alternative definition of 'intercalation' applies in some other fields of chemistry.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1991

intercalation reaction

Also contains definition of: insertion reaction

Reaction, generally reversible, that involves the penetration of a host material by guest species without causing a major structural modification of the host.
Notes:

1. Intercalation can refer to the insertion of a guest species into a one-, two- or three-dimensional host structure.
2. The guest species is not distributed randomly but occupies positions predetermined by the structure of the host material.
3. Examples of intercalation reactions are the insertion of lithium into layered TiS_2 [Li_xTiS_2 ($0 \leq x \leq 1$)] and of potassium into the layers of graphite (C_8K).

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1823

interchange reaction

Reaction that results in an exchange of atoms or groups between a polymer and low-molar-mass molecules, between polymer molecules, or between sites within the same macromolecule.
Note:
An interchange reaction that occurs with polyesters is called transesterification.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 892

interchromophoric radiationless transition

See: radiationless transition

Source:
Orange Book, p. 187

interconal region

The region of a Bunsen flame where the combustion zone has the form of a cone.

Source:
Orange Book, p. 166

interconvertible enzyme

An enzyme existing in at least two well defined, reversibly convertible forms, produced by covalent modifications of amino acid side chains under biological conditions. Covalent modifications that occur as intermediates in the catalytic process are not included in this definition.

Source:
White Book, p. 94

interface

The plane ideally marking the boundary between two phases.
Note:
The term should not be used synonymously with interphase.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

See also:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 583
Orange Book, p. 251

interfacial adhesion

Adhesion in which interfaces between phases or components are maintained by intermolecular forces, chain entanglements, or both, across the interfaces.
Notes:

1. Interfacial adhesion is also referred to as tack.
2. Adhesive strength (recommended symbol: F_a, unit: $\mathrm{N\ m^{-2}}$) is the force required to separate one condensed phase domain from another at the interface between the two phase domains divided by the area of the interface.
3. Interfacial tension (recommended symbol: γ, unit: $\mathrm{N\ m^{-1}}$, $\mathrm{J\ m^{-2}}$) is the change in Gibbs energy per unit change in interfacial area for substances in physical contact.
4. Use of the term interfacial energy for interfacial tension is not recommended.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1992

interfacial concentration, *c*

in electrochemistry

The interfacial concentration $c_{B,e}$ (or simply c_e) of a species **B** is the concentration of that species at the boundary of the electrical double-layer facing the solution, i.e. just outside the region where the departures from the electroneutrality of the solution are significant. This concept is mainly used in the usual case where the thickness of the electric double layer is very small as compared to that of the diffusion layer. It is often calculated from theory or derived from measurements of the limiting current.
See: mass transfer coefficient *in electrochemistry*

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1837

See also:
PAC, 1980, *52*, 233 *(Electrode reaction orders, transfer coefficients and rate constants. Amplification of definitions and recommendations for publication of parameters)* on page 236

interfacial double-layer

Also contains definitions of: electrical double-layer, surface charge layer, transition layer

The Coulombic interaction of interfacial charges (e.g. ions) and the magnetic or electrostatic interaction of interfacial molecules lead to particularly complex interfacial structures. Complex interfacial profiles that can be approximated by two distinct sub-layers with different physical properties (e.g. structure and/or nature and/or composition), are referred to as interfacial double-layers. Examples of such approximated complex profiles are: the electrical double-layer consisting of a surface charge layer (i.e. a two dimensional distribution of one type of ions) and a diffuse charge layer (counter-ions distributed over the space region next to the surface); the approximated profile of the orientation angle of anisotropic liquid molecules within a 'double-layer' consisting of a distribution of so-called anchored molecules which are perturbed (strongly bound and orientated) by the surface, and the adjacent, so-called, transition layer, i.e. the region where the surface perturbation is damped.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1674

interfacial layer

The inhomogeneous space region intermediate between two bulk phases in contact, and where properties are significantly different from, but related to, the properties of the bulk phases. Examples of such properties are: compositions, molecular density, orientation or conformation, charge density, pressure tensor, electron density, etc. The interfacial properties vary in the direction normal to the surface. Complex profiles of interfacial properties occur in the case of multicomponent systems with coexisting bulk phases where attractive/repulsive molecular interactions involve adsorption or depletion of one or several components. This interfacial region may also be regarded as a distinct, though not autonomous, phase and be called the interphase.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1673
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

interfacial layer width, σ_{S}

in thin films

The characteristic length defined by the variance of the Gaussian function fitted to the gradient of the electron density profile established by X-ray specular reflectivity studies of the liquid interface.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1674

interfacial region

See: interfacial layer

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1673
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

interfacial tension

See: surface tension

Source:
Green Book, 2nd ed., p. 12
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 596

interference

in analysis

A systematic error in the measure of a signal caused by the presence of concomitants in a sample.

Source:
PAC, 1983, *55*, 553 *(Recommendations for the usage of selective, selectivity and related terms in analytical chemistry)* on page 554

interfering lines

Radiation from nearby spectral lines may perturb the measurement of the intensity of the line wanted. These lines are termed interfering lines.

Source:
Orange Book, p. 159

interfering substance

in electroanalytical chemistry

Any substance, other than the ion being measured, whose presence in the sample solution affects the measured emf of a cell. Interfering substances fall into two classes: 'electrode/electrochemical' interferences and 'chemical' interferences. Examples of the first class include:

1. Those substances which give a similar response to the ion being measured and whose presence generally results in an apparent increase in the activity (or concentration) of the ion to be determined (e.g. Na^+ for the Ca^{2+} electrode).
2. Electrolytes present at a high concentration that give rise to appreciable liquid junction potential differences or results in a significant activity coefficient decrease, or incipient Donnan exclusion failure. The second class of substances that should be recognized as chemical interferences includes:
3. Species that interact with the ion being measured so as to decrease its activity or apparent concentration. The electrode continues to report the true activity (e.g. CN^- present in the measurement of Ag^+), but a considerable gap will occur between the activity and concentration of the ions even in very dilute solutions. Under these circumstances the determination of ionic concentration may be problematic.
4. Substances interacting with the membrane itself, blocking the surface or changing its chemical composition [i.e. organic solvents for the liquid or poly(vinyl chloride) (PVC) membrane electrodes] are grouped as interferences or electrode poisons.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2530

interferometer

See: Fourier transform spectrometer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2248

interferons

A class of glycoproteins (with sugar groups attached at specific locations) important in immune function. They are able to inhibit the multiplication of viruses in cells.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

intermediate

A molecular entity with a lifetime appreciably longer than a molecular vibration (corresponding to a local potential energy minimum of depth greater than $R\,T$) that is formed (directly or indirectly) from the reactants and reacts further to give (either directly or indirectly) the products of a chemical reaction; also the corresponding chemical species.
See: reaction step, elementary reaction, stepwise reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1126

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 170

intermediate neutrons

Neutrons of kinetic energy between the energies of slow and fast neutrons. In reactor physics, the range might be $1\ \mathrm{eV}$ to $0.1\ \mathrm{MeV}$.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

intermolecular

1. Descriptive of any process that involves a transfer (of atoms, groups, electrons, etc.) or interactions between two or more molecular entities.
2. Relating to a comparison between different molecular entities.
   See also: intramolecular

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1126

intermolecular radiationless transition

See: radiative transition

Source:
Orange Book, p. 185

internal absorptance, α_i

Absorptance when surface effects and effects of the cuvette such as reflection losses are excluded.

Source:
Green Book, 2nd ed., p. 32

internal compensation [obsolete]

Usage strongly discouraged.
See: meso-compound

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

internal conversion

A photophysical process. An isoenenergetic radiationless transition between two electronic states of the same multiplicity. When the transition results in a vibrationally excited molecular entity in the lower electronic state, this usually undergoes deactivation to its lowest vibrational level, provided the final state is not unstable to dissociation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2248

See also:
Orange Book, p. 187
Orange Book, p. 216

internal energy, *U*

Synonym: thermodynamic energy

Quantity the change in which is equal to the sum of heat, q, brought to the system and work, w, performed on it, $\Delta U = q + w$. Also called thermodynamic energy.

Source:
Green Book, 2nd ed., p. 48
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 976

internal filling solution

of a glass electrode

Aqueous electrolyte solution, which may be gelled, containing fixed concentration of hydrogen ions, e.g. HCl or a buffer solution, and a fixed concentration of the ion to which the internal reference electrode is reversible, e.g. chloride ion in the case of silver-silver chloride, or calomel electrodes.

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 540

internal reference electrode

An 'inner' reference electrode which is contained inside an ion-selective electrode assembly.
Note:
The system frequently consists of a silver/silver chloride electrode in contact with an appropriate solution containing fixed concentrations of chloride and the ion for which the membrane is selective. This 'inner' filling solution is in contact with the ion-selective membrane.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2533

internal standard

in chromatography

A compound added to a sample in known concentration to facilitate the qualitative indentification and/or quantitative determination of the sample components.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 837

internal surface

With respect to porous solids, the surface associated with pores communicating with the outside space. Since the accessibility of pores may depend on the size of the fluid molecules, the extent of the accessible internal surface may depend on the size of the molecules comprising the fluid, and may be different for the various components of a fluid mixture (molecular sieve effect).

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 585

internal valence force field

Acronym: IVFF

A force field expressed in terms of bond-stretching, angle-bending, torsional and other displacements directly connected to the structural parameters of the molecule:

$$V = \frac{1}{2} \sum k_{ij} R_i R_j$$

or

$$V = \frac{1}{2} \sum K_{ij} R_i R_j$$

where k (or K) are the force constants and R the internal valence coordinates.

Source:
PAC, 1978, *50*, 1707 *(Definition and symbolism of molecular force constants)* on page 1709

international calorie

See: calorie

Source:
Green Book, 2nd ed., p. 112
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 976

international unit **[obsolete]**

The unit of enzyme activity proposed by the International Union of Biochemistry in 1964. Specifically, it is the amount of enzyme that catalyses the conversion of one micromole of substrate per minute under the specified conditions of the assay method.
Note:
This unit is no longer recommended because the term does not indicate what physical quantity it refers to, and because the minute is not the SI unit of time.

Source:
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

interparticle porosity, ε

in chromatography

The interparticle volume of a packed column per unit column volume:

$$\varepsilon = \frac{V_0}{V_c}$$

It is also called the interstitial fraction of the column.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 832

interparticle volume of the column, V_0

in chromatography

The volume occupied by the mobile phase between the particles in the packed section of a column. It is also called the interstitial volume or the void volume of the column. In liquid chromatography, the interparticle volume is equal to the mobile-phase hold-up volume (V_M) in the ideal case, neglecting any extra-column volume. In gas chromatography, the symbol V_G may be used for the interparticle volume of the column. In the ideal case, neglecting any extra-column volume, V_G is equal to the corrected gas hold-up volume (V_M^o).

$$V_G = V_M^o = V_{M\,j}$$

interpenetrating polymer network

Acronym: IPN

Polymer comprising two or more networks that are at least partially interlaced on a molecular scale but not covalently bonded to each other and cannot be separated unless chemical bonds are broken.
Note:
A mixture of two or more preformed polymer networks is not an IPN.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1814

interphase

See: interfacial layer

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1673

interphase transition

A transition that occurs at boundaries between phases. Example: The precipitation of second phases or the initiation of new phase growth at an interface.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 584

intersection space

($3N - 8$)-dimensional subspace of the ($3N - 6$)-dimensional nuclear coordinate space consisting of an infinite number of conical intersection points (N is the number of nuclei).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 356

interstitial fraction

in chromatography

The interstitial volume per unit volume of a packed column. Defined by:

$$\varepsilon_{\mathrm{I}} = \frac{V_{\mathrm{I}}}{X}$$

where V_{I} is the interstitial volume and X the column volume.

Source:
Orange Book, p. 100

interstitial velocity

in chromatography

The linear velocity of the mobile phase inside a packed column calculated as the average over the entire cross section. This quantity can, under idealized conditions, be calculated from the equation:

$$u = \frac{F}{\varepsilon_{\mathrm{I}}}$$

where F is the nominal linear flow and ε_{I} the interstitial fraction

Source:
Orange Book, p. 102

interstitial volume

in gas chromatography

The volume V_{G} of the column not occupied by the liquid phase and its solid support, or by the active solid. It does not include any volume external to the column, such as the volume of the sample injector or of the detector.

Source:
Orange Book, p. 99

intersystem crossing

A photophysical process. An isoenergetic radiationless transition between two electronic states having different multiplicities. It often results in a vibrationally excited molecular entity in the lower electronic state, which then usually deactivates to its lowest vibrational level.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2248

See also:
Orange Book, p. 187

interval analysis

A method to estimate uncertainties in the results of a least-squares procedure. The input data are primary values plus limits of intervals expressing their uncertainty. The output consists of derived values plus limits of intervals expressing a pessimistic estimate of maximal uncertainty.

Source:
PAC, 1981, *53*, 1805 *(Assignment and presentation of uncertainties of the numerical results of thermodynamic measurements (Provisional))* on page 1823

intervalence charge transfer

Electron transfer (thermal or photoinduced) between two metal sites differing only in oxidation state. Quite often such electron transfer reverses the oxidation states of the sites. The term is frequently extended to the case of metal-to-metal charge transfer between non-equivalent metal centres.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2248

interzonal region

The region of the Bunsen flame confined by the inner and outer zones, where in many instances the conditions for flame analysis are optimum.

Source:
Orange Book, p. 166

intra-

in organic reaction mechanisms

The prefix for an elementary reaction or some part thereof indicating that the bond(s) undergoing primitive changes form part of a ring in the transition state of the elementary reaction. This prefix is used for nonpericyclic processes only and is replaced by 'cyclo' for pericyclic processes.

Source:
PAC, 1989, *61*, 23 *(System for symbolic representation of reaction mechanisms (Recommendations 1988))* on page 34

intrachromophoric radiationless transition

See: radiationless transition

Source:
Orange Book, p. 187

intramolecular

1. Descriptive of any process that involves a transfer (of atoms, groups, electrons, etc.) or interactions between different parts of the same molecular entity.
2. Relating to a comparison between atoms or groups within the same molecular entity.

See also: intermolecular

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1126

intramolecular catalysis

The acceleration of a chemical transformation at one site of a molecular entity through the involvement of another functional ('catalytic') group in the same molecular entity, without that group appearing to have undergone change in the reaction product. The use of the term should be restricted to cases for which analogous intermolecular catalysis by chemical species bearing that catalytic group is observable. Intramolecular catalysis can be detected and expressed in quantitative form by a comparison of the reaction rate with that of a comparable model compound in which the catalytic group is absent, or by measurement of the effective molarity of the catalytic group.
See also: neighbouring group participation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1126

intramolecular charge transfer, (ICT)

Process that changes the overall charge distribution in a molecule.
Note:
For intramolecular charge transfer in the excited state, several models are discussed in the literature based on the molecular structure of the final state reached upon photo-induced ICT: planar intramolecular charge transfer (PICT) or twisted intramolecular charge transfer (TICT). For example, an ICT has been proposed to be responsible for the strongly Stokes-shifted additional fluorescence band in fluorescent molecules with two fluorescence bands (dual fluorescent molecules).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 357

intramolecular isotope effect

A kinetic isotopic effect observed when a single substrate, in which the isotopic atoms occupy equivalent reactive positions, reacts to produce a non-statistical distribution of isotopomeric products. In such a case the isotope effect will favour the pathway with lower force constants for displacement of the isotopic nuclei in the transition state.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1130

intraphase transition

A transition that occurs within a phase. Example: Initiation of phase growth at an intragranular feature, such as twin planes and dislocations in steels.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 584

intrinsic activation energy, $E_{\mathrm{a,i}}$

If $E_{\mathrm{a,1}}$ and $E_{\mathrm{a,-1}}$ are the activation energies for a reaction in forward and reverse directions, the lesser of the two is sometimes called the intrinsic activation energy. It is the activation energy for the reaction in the exothermic direction.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 170

intrinsic barrier

The Gibbs energy of activation ($\Delta^{\ddagger}G$) in the limiting case where $\Delta G^{\circ} = 0$, i.e. when the effect of thermodynamic driving force is eliminated. According to the Marcus equation, the intrinsic barrier is related to the reorganization energy, λ, of the reaction by the equation:

$$\Delta^{\ddagger}G = \frac{\lambda}{4}$$

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1126

intrinsic detector efficiency

The ratio of the number of particles or photons detected to the number of similar particles or photons which have struck the envelope limiting the sensitive volume of a radiation detector.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518

intrinsic full energy peak efficiency

The detector efficiency when considering only events where the total energy of the radiation is absorbed in the sensitive volume of the detector.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

intrinsic photopeak efficiency

The detector efficiency when only counts resulting from the photoelectrical effect are considered.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

intrinsic reaction coordinate

A minimum-energy reaction path on a potential energy surface in mass-weighted coordinates, connecting reactants to products *via* the transition state.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1947

intrinsic viscosity
Synonym: limiting viscosity number

of a polymer

The limiting value of the reduced viscosity, $\frac{\eta_{\mathrm{i}}}{c}$ or the inherent viscosity, η_{inh}, at infinite dilution of the polymer, i.e.

$$[\eta] = \lim_{c \to 0} \frac{\eta_{\mathrm{i}}}{c} = \lim_{c \to 0} \eta_{\mathrm{inh}}$$

Notes:
1. This term is also known in the literature as the Staudinger index.
2. The unit must be specified; $\mathrm{cm}^3\ \mathrm{g}^{-1}$ is recommended.
3. This quantity is neither a viscosity nor a pure number. The term is to be looked on as a traditional name. Any replacement by consistent terminology would produce unnecessary confusion in the polymer literature. Synonymous with limiting viscosity number.

Source:
Purple Book, p. 63

intrinsically conducting polymer

Electrically conducting polymer composed of macromolecules having fully conjugated sequences of double bonds along the chains.

Notes:

1. The bulk electrical conductivity of an intrinsically conducting polymer is comparable to that of some metals and results from its macromolecules acquiring positive or negative charges through oxidation or reduction by an electron-acceptor or -donor (charge-transfer agent), termed a dopant.
2. Examples of intrinsically conducting polymers are polyacetylene, polythiophene, polypyrrole, or polyaniline. Unlike polymeric electrolytes, in which charge is transported by dissolved ions, charge in intrinsically conducting polymers is transported along and between polymer molecules via generated charge carriers (e.g., holes, electrons).
3. An intrinsically conducting polymer should be distinguished from a conducting polymer composite and from a solid polymer electrolyte.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2070

intron

An intervening section of DNA occuring almost exclusively within a eukaryotic gene but which is not translated to amino acid sequences in the gene product. The introns are removed from the premature mRNA through a process called splicing to form an active mRNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

inverse isotope effect

A kinetic isotope effect in which $\frac{k^{\mathrm{l}}}{k^{\mathrm{h}}} < 1$, i.e. the heavier substrate reacts more rapidly than the lighter one, as opposed to the more usual 'normal' isotope effect, in which $\frac{k^{\mathrm{l}}}{k^{\mathrm{h}}} > 1$. The isotope effect will normally be 'normal' when the frequency differences between the isotopic transition states are smaller than in the reactants. Conversely, an inverse isotope effect can be taken as evidence for an increase in the corresponding force constants on passing from the reactant to the transition state.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1130

inverse kinetic isotope effect

See: isotope effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1126

inverse square law

in radiation chemistry

The intensity of radiation from a point source in free space is inversely proportional to the square of the distance from the source. Presence of absorbers necessitates corrections to this law.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1544

inversion

1. ***See:*** Walden inversion
2. ***See:*** pyramidal inversion
3. ***See:*** ring inversion
4. A symmetry operation involving a centre of inversion (i).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

inversion height

in atmospheric chemistry

The height above ground level at which there is change in sign of the normal temperature 'lapse rate', $\frac{\mathrm{d}T}{\mathrm{d}z}$ (the rate of change of the temperature with height). Several temperature inversions may be present in the air over a given site at different altitudes as result of various meteorological factors.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2197

inversion point

in phase transitions

The temperature (pressure) at which one polymorph of a solid phase changes into another at constant pressure (temperature).
See: polymorphic transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 584

inverted micelle

Synonyms: inverse micelle, reverse micelle (or reversed micelle)

The reversible formation of association colloids from surfactants in non-polar solvents leads to aggregates termed inverted (or inverse, reverse or reversed) micelles. Such association is often of the type:

$$\text{Monomer} \rightleftarrows \text{Dimer} \rightleftarrows \text{Trimer} \rightleftarrows \ldots n-\text{mer}$$

and the phenomenon of critical micelle concentration (or an analogous effect) is consequently not observed. In an inverted micelle the polar groups of the surfactants are concentrated in the interior and the lipophilic groups extend towards and into the non-polar solvent.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1126

inverted region (for electron transfer)

In plots relating rate constants to charges in standard Gibbs energy (ΔG°) for electron transfer a region may occur in which the rate constants decrease as the exergonicity of the reaction increases. This region is often referred to as the inverted region and its presence is predicted by the theory developed for outer sphere electron transfer for the case $-\Delta G^\circ > \lambda$ in the Marcus equation, λ being the reorganization energy. Note the similarity to the energy gap law for radiationless conversion of an excited state.
See: normal region

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2249

iodohydrins

See: halohydrins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

iodometric titration

See: titration

Source:
Orange Book, p. 47

ion

An atomic or molecular particle having a net electric charge.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1545

ion collector

in mass spectrometry

Device for the capture of selected ions such as a Faraday cup collector (with a d.c. amplifier) or an electron multiplier.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

ion cyclotron resonance (ICR) mass spectrometer

A high-frequency mass spectrometer in which the ions to be detected, with a selected value of the quotient mass/charge, absorb maximum energy through the effect of a high-frequency electric field and a constant magnetic field perpendicular to the electric field. Maximum energy is gained by the ions which satisfy the cyclotron resonance condition and as a result they are separated from ions of different mass/charge.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545
Orange Book, p. 202

ion energy loss spectra

in mass spectrometry

Spectra that show the loss of translational energy of ions involved in ion/neutral species reactions.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

ion exchange

1. In surface chemistry, if the adsorption of one or several ionic species is accompanied by the simultaneous desorption (displacement) of an equivalent amount of one or more other ionic species, this process is called ion exchange.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 585

2. The process of exchanging ions between a solution and an ion exchanger.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 854

ion exchanger

A solid or liquid, inorganic or organic substance containing exchangeable ions with others of the same charge, present in a solution in which the ion exchanger is considered to be insoluble. It is recognized that there are cases where liquid exchangers are employed and where it may be difficult to distinguish between the separation process as belonging to ion exchange or liquid-liquid distribution, but the broad definition given here is regarded as that which is most appropriate. A monofunctional ion exchanger contains only one type of ionogenic group, a bifunctional ion exchanger two types and a polyfunctional ion exchanger more than one type. In a macroporous ion exchanger the pores are large compared to atomic dimensions.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 855

ion kinetic energy spectrum

in mass spectrometry

A spectrum obtained when a beam of ions is separated according to the translational energy-to-charge ratios of the ionic species contained within it. A radial electric field (E) achieves separation of the various ionic species in this way.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

ion laser

A gas laser in which the active species is an ion formed in the electric discharge. Most practically important lasers of this type have continuous wave (CW) output. Examples are the argon ion, krypton ion and helium-cadmium (HeCd) lasers.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1920

ion microscopy

Use of the secondary ion mass spectrometry (SIMS) technique to obtain micrographs of the elemental (or isotopic) distribution at the surface of a sample with a spatial resolution of $2\ \mu\text{m}$ or better.

Source:
Orange Book, p. 249

ion pair

Also contains definitions of: contact ion pair, intimate ion pair, loose ion pair, solvent-separated ion pair, solvent-shared ion pair, tight ion pair

A pair of oppositely charged ions held together by Coulomb attraction without formation of a covalent bond. Experimentally, an ion pair behaves as one unit in determining conductivity, kinetic behaviour, osmotic properties, etc. Following Bjerrum, oppositely charged ions with their centres closer together than a distance:

$$q = \frac{8.36 \times 10^6\, z^+ z^-}{\varepsilon_\mathrm{r}\, T}\ \mathrm{pm}$$

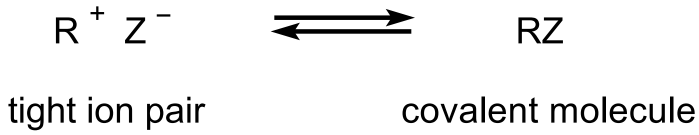
are considered to constitute an ion pair ('Bjerrum ion pair'). [z^+ and z^- are the charge numbers of the ions, and ε_r is the relative permittivity (or dielectric constant) of the medium.] An ion pair, the constituent ions of which are in direct contact (and not separated by an intervening solvent or other neutral molecule) is designated as a 'tight ion pair' (or 'intimate' or 'contact ion pair'). A tight ion pair of X^+ and Y^- is symbolically represented as X^+Y^-. By contrast, an ion pair whose constituent ions are separated by one or several solvent or other neutral molecules is described as a 'loose ion pair', symbolically represented as $X^+ \parallel Y^-$. The members of a loose ion pair can readily interchange with other free or loosely paired ions in the solution. This interchange may be detectable (e.g. by isotopic labelling) and thus afford an experimental distinction between tight and loose ion pairs. A further conceptual distinction has sometimes been made between two types of loose ion pairs. In 'solvent-shared ion pairs' the ionic constituents of the pair are separated by only a single solvent molecule, whereas in 'solvent-separated ion pairs' more than one solvent molecule intervenes. However, the term 'solvent-separated ion pair' must be used and interpreted with care since it has also widely been used as a less specific term for 'loose' ion pair.
See also: common-ion effect, dissociation, ion-pair return, special salt effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1126
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

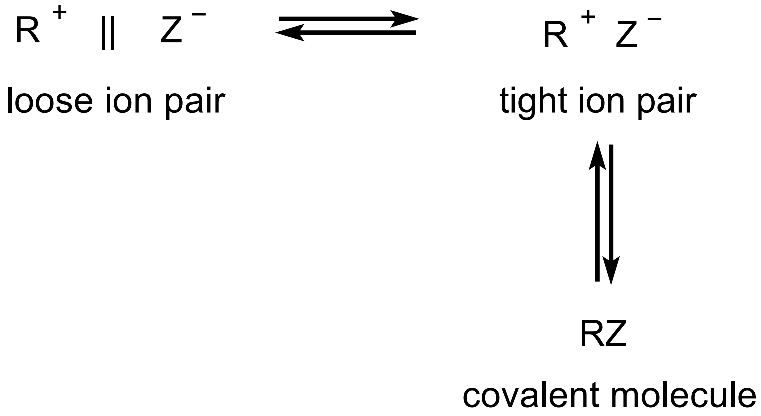
ion pair return

Also contains definitions of: external ion-pair return, hidden return, internal return

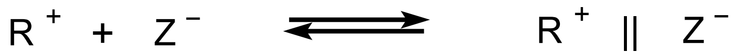
The recombination of a pair of ions R^+ and Z^- formed from ionization of RZ. If the ions are paired as a tight ion pair and recombine without prior separation into a loose ion pair this is called 'internal ion-pair return':



It is a special case of 'primary geminate recombination'. If the ions are paired as a loose ion pair and form the covalent chemical species via a tight ion pair, this is called 'external ion-pair return':



It is a special case of 'secondary geminate recombination'. When the covalent molecule RZ is reformed without direct evidence of prior partial racemization or without other direct evidence of prior formation of a tight ion pair, (e.g. without partial racemization if the group R is suitably chiral) the internal ion-pair return is sometimes called a 'hidden return'. External (unimolecular) ion-pair return is to be distinguished from 'external (bimolecular) ion return', the (reversible) process whereby dissociated ions are converted into loose ion pairs:



Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1127

ion probe microanalysis (IPMA)

Any technique in which the specimen is bombarded by a focused beam of (primary) ions (diameter less than $10\ \mu m$) and the (secondary) ions ejected from the specimen are detected after passage through a mass spectrometer.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2025
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2246

ion pumps

Ion pumps enable ions to flow through membranes in a thermodynamically uphill direction by the use of an energy source such as ATP or light. They consist of sugar-containing hetero-peptide assemblies, which open and close upon the binding and subsequent hydrolysis of ATP, usually transporting more than one ion towards the outside or the inside of the membrane.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1281

ion scattering spectrometry (ISS)

Any technique using low energy $(10\ \mathrm{keV})$ ions in which the bombarding particles scattered by the sample are detected and recorded as a function of energy and/or angle. This technique is used mainly for determining the composition and structure of the first few atomic layers of a sample.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2246

ion source

in mass spectrometry

Generally an assembly composed of: (i) an ionization chamber in which a stream of electrons flows from a hot filament across a stream of gas to collector (the potential between filament and collector is usually between 50 and 70 V); (ii) a device for the acceleration of these ions.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

ion trap mass spectrometer

An arrangement in which ions with a desired range of quotients mass/charge are first made to describe stable paths under the effect of a high-frequency electric quadrupole field, and are then separated and presented to a detector by adjusting the field so as to selectivity induce path instability according to their respective mass/charge ratios.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545

ion-exchange chromatography

Chromatography in which separation is based mainly on differences in the ion-exchange affinities of the sample components. Present day ion-exchange chromatography on small particle high efficiency columns and usually utilizing conductometric or spectroscopic detectors is often referred to as ion chromatography (IC).

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 826

ion-exchange isotherm

The concentration of a counter-ion in the ion exchanger expressed as a function of its concentration in the external solution under specified conditions and at constant temperature.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 854

ion-exchange polymer

Also contains definition of: ion-exchange membrane

Polymer that is able to exchange ions (cations or anions) with ionic components in solution.
Notes:

1. ***See also:*** ion exchange.
2. An ion-exchange polymer in ionized form may also be referred to as a polyanion or a polycation.
3. Synthetic ion-exchange organic polymers are often network polyelectrolytes.
4. A membrane having ion-exchange groups is called an ion-exchange membrane.
5. Use of the term 'ion-exchange resin' for 'ion-exchange polymer' is strongly discouraged.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 895

ion-free layer

An interphase in which only non-specifically adsorbed ions are present.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1261

ion-pair formation

in mass spectrometry

Involves an ionization process in which a positive fragment ion and a negative fragment ion are among the products.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548

ion-selective electrode cell

An ion-selective electrode in conjunction with a reference electrode. Generally, the cell contains two reference electrodes, internal and external, and the thin film or membrane recognition-transduction element. However, besides this conventional type of cell (with solution contact on both sides of the membrane) there are cell arrangements with wire contact to one side of the membrane (all solid state and coated wire types).

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2531

ion-selective electrode (ISE)

An electrochemical sensor, based on thin films or selective membranes as recognition elements, and an electrochemical half-cell equivalent to other half-cells of the zeroth (inert metal in a redox electrolyte), 1st, 2nd and 3rd kinds. These devices are distinct from systems that involve redox reactions (electrodes of zeroth, 1st, 2nd and 3rd kinds), although they often contain a 2nd kind electrode as the 'inner' or 'internal' reference electrode. The potential difference response has, as its principal component, the Gibbs energy change associated with permselective mass transfer (by ion-exchange, solvent extraction or some other mechanism) across a phase boundary. The ion-selective electrode must be used in conjunction with a reference electrode (i.e. 'outer' or 'external' reference electrode) to form a complete electrochemical cell. The measured potential differences (ion-selective electrode vs. outer reference electrode potentials) are linearly dependent on the logarithm of the activity of a given ion in solution. Comment: The term 'ion-specific electrode' is not recommended. The term 'specific' implies that the electrode does not respond to additional ions. Since no electrode is truly specific for one ion, the term 'ion-selective' is recommended as more appropriate. 'Selective ion-sensitive electrode' is a little-used term to describe an ion-selective electrode. 'Principal' or 'primary' ions are those which an electrode is designed to measure. It is never certain that the 'principal' ion is most sensitively measured, e.g. nitrate ion-selective electrodes.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2531

ion/molecule reaction

in mass spectrometry

An ion/neutral species reaction in which the neutral species is a molecule. The use of ion-molecule reaction is not recommended; the hyphen suggests a reaction of a species that is both an ion and a molecule and is not the intended meaning.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1556
Orange Book, p. 206

ion/neutral species exchange reaction

in mass spectrometry

In this reaction an association reaction is accompanied by the subsequent or simultaneous liberation of a different neutral species as product.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1556

ion/neutral species reaction

in mass spectrometry

A process wherein a charged species interacts with a neutral reactant to produce either chemically different species or changes in the internal energy of one or both of the reactants. The contrasting expression ion/neutral reaction is not ideal, simply because the word neutral is not a noun. However, any alternatives such as ion/neutral species reaction are so clumsy as to mitigate against their general acceptance

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1556

ionene

Polymer composed of macromolecules in which ionized or ionic groups are parts of main chains.
Note:
Most commonly, the ionic groups in ionenes are quaternary ammonium groups.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2071

ionic aggregates in an ionomer

Domains enriched with ionic groups within an ionomer matrix.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2071

ionic bond

The bond between atoms with sharply different electronegativities. In strict terms, an ionic bond refers to the electrostatic attraction experienced between the electric charges of a cation and an anion, in contrast with a purely covalent bond. In practice, it is preferable to consider the amount of ionic character of a bond rather than referring to purely ionic or purely covalent bonds. The relationship was proposed (L. Pauling) for the estimation of ionic character of a bond between atoms A and B:

$$\text{Amount of ionic character} = 1 - e^{-1/4}\,(\chi_{\mathrm{A}} - \chi_{\mathrm{B}})$$

where χ_{A} and χ_{B} are the Pauling electronegativities of atoms A and B. This type of bonding is realized mostly in solids.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1947

ionic concentration

See: concentration

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 977

ionic conductivity

Defined for ionic species B by

$$\lambda = |z_{\mathrm{B}}|\, F\, u_{\mathrm{B}}$$

where z_{B} is the charge number of the ionic species B, F is the Faraday constant, and u_{B} is the electric mobility of species B. In most current practice z_{B} is taken as unity, i.e. ionic conductivity is taken as that of species such as Na^{+}, $\mathrm{Ca}^{2+}/2$, $\mathrm{La}^{3+}/3$ etc. To avoid ambiguity the species considered should be clearly stated, e.g. as $\lambda(\mathrm{Ca}^{2+}/2)$.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 512

ionic copolymerization

A copolymerization which is an ionic polymerization.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2308

ionic dissociation

in mass spectrometry

The decomposition of an ion into another ion of lower mass and one or more neutral species.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1547

ionic polymer

Synonym: ion-containing polymer

Polymer composed of macromolecules containing ionic or ionizable groups, or both, irrespective of their nature, content, and location.
Synonym: ion-containing polymer.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2071

ionic polymerization

A chain polymerization in which the kinetic-chain carriers are ions or ion pairs.
Note:
Usually, the growing chain ends are ions.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2308

ionic strength, I

On a molality basis,

$$I_m = \frac{1}{2} \sum m_{\mathrm{B}}\, z_{\mathrm{B}}^2$$

where the sum goes over all the ions B. z_{B} is the charge number of ion B. The ionic strength on a concentration basis is defined analogously

$$I_c = \frac{1}{2} \sum c_{\mathrm{B}}\, z_{\mathrm{B}}^2.$$

Source:
Green Book, 2nd ed., p. 50
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 977

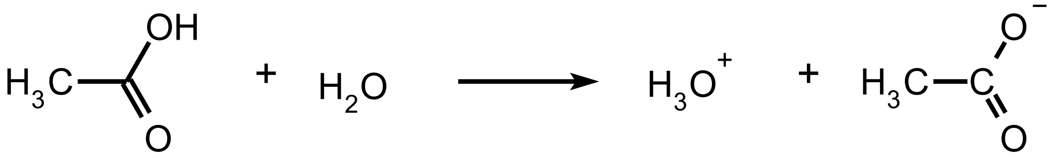
ionic transport number, *t*

Quotient of the current carried by an ionic component and the total current.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 977

ionization

The generation of one or more ions. It may occur, e.g. by loss of an electron from a neutral molecular entity, by the unimolecular heterolysis of such an entity into two or more ions, or by a heterolytic substitution reaction involving neutral molecules, such as:



$$Ph_3CCl + AlCl_3 \longrightarrow Ph_3C^+ + AlCl_4^-$$

(electrophile assisted)

$$Ph_3CCl \longrightarrow Ph_3C^+\ Cl^-$$

(ion pair, in benzene)

The loss of an electron from a singly, doubly, etc. charged cation is called second, third, etc. ionization. This terminology is used especially in mass spectroscopy.
See also: dissociation, ionization energy

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1127

ionization buffer

in flame spectroscopy

A buffer added to increase the free-electron concentration by the flame gases, thus repressing and stabilizing the degree of ionization.

Source:
Orange Book, p. 172

ionization by sputtering

Ionization by bombardment of a solid specimen with accelerated ions or electrons or fast neutrals.

Source:
Orange Book, p. 204

ionization chamber

A radiation detector which employs an electric field for the collection at the electrodes of charges associated with the ions produced in the sensitive volume by ionizing radiation, without charge multiplication. The solid angle (2Π, 4π) subtended when using the detector, is sometimes specified.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1545

ionization cross-section

A measure of the probability that a given ionization process will occur when an atom or molecule interacts with an electron or a photon.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548

ionization efficiency

The ratio of the number of ions formed to the number of electrons or photons used in an ionization process.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548

ionization efficiency curve

in mass spectrometry

The number of ions produced as a function of the energy of the electrons or photons used to produce ionization.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548
Orange Book, p. 206

ionization energy, E_i

Minimum energy required to eject an electron out of a neutral atom or molecule in its ground state. The adiabatic ionization energy refers to the formation of the molecular ion in its ground vibrational state and the vertical ionization energy applies to the transition to the molecular ion without change in geometry. This quantity was formerly called ionization potential. The second ionization energy of an atom is the energy required to eject the second electron from the atom (energy for the process

$X^{+} \longrightarrow X^{2+} + e$).

Source:
Green Book, 2nd ed., p. 20
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1128

ionization potential **[obsolete]**

See: ionization energy

Source:
Green Book, 2nd ed., p. 20

ionizing collision

in mass spectrometry

An ion/neutral species interaction in which an electron or electrons are stripped from the ion and/or the neutral species in the collision. Generally, this term has come to be used to describe collisions of fast-moving ions with a neutral species in which the neutral species is ionized with no change in the number of charges carried by the ion. Care should be taken when this term is used to emphasize if charge stripping of the ion has taken place.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1555

ionizing power

A term to denote the tendency of a particular solvent to promote ionization of an uncharged or, less often, charged solute. The term has been used both in a kinetic and in a thermodynamic context.
See also: Dimroth–Reichardt E_T parameter, Grunwald–Winstein equation, Z-value

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1128

ionizing radiation

Any radiation consisting of directly or indirectly ionizing particles or a mixture of both, or photons with energy higher than the energy of photons of ultraviolet light or a mixture of both such particles and photons.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

ionizing voltage

The voltage difference through which electrons are accelerated before they are used to bring about electron impact ionization. To obtain the true ionizing voltage, corrections for any contact or surface potentials must be made.
Note:
The term electron energy is frequently used in place of ionizing voltage.

Source:
Orange Book, p. 203

ionogenic groups

The fixed groupings in an ion exchanger which are either ionized or capable of dissociation into fixed ions and mobile counter-ions.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 854

ionomer

Polymer composed of macromolecules in which a small but significant proportion of the constitutional units has ionic or ionizable groups, or both.
Note:
Ionic groups are usually present in sufficient amounts (typically less than 10% of constitutional units) to cause micro-phase separation of ionic domains from the continuous polymer phase. The ionic domains act as physical crosslinks.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2071

ionomer cluster

Ionic aggregate, in a polymer matrix of low polarity, formed through interactions of ionomer multiplets.
Notes:

1. The mobility of the polymer segments surrounding the multiplets is reduced relative to that of bulk material. With increasing ion content, the number density of the ionomer multiplets increases, leading to overlapping of the restricted mobility regions around the multiplets and the formation of clusters.
2. Typically, an ionomer exhibits two glass transition temperatures (T_g), one for the non-polar matrix and the other for clusters.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2072

ionomer molecule

A macromolecule in which a small but significant proportion of the constitutional units have ionizable or ionic groups, or both. Some protein molecules may be classified as ionomer molecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2299

ionomer multiplet

Ionic aggregate, in a polymer matrix of low polarity, formed through the association of ion-pairs in an ionomer.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2072

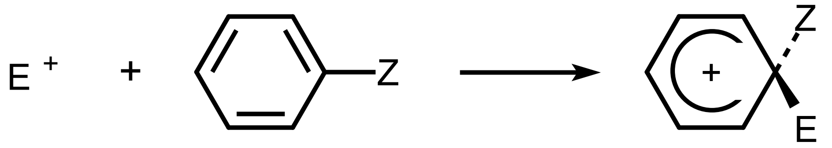
ionophore

A compound which can carry specific ions through membranes of cells or organelles.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1280

ipso-attack

The attachment of an entering group to a position in an aromatic compound already carrying a substituent group (other than hydrogen). The entering group may displace that substituent group but may also itself be expelled or migrate to a different position in a subsequent step. The term '*ipso*-substitution' is not used, since it is synonymous with substitution. For example:

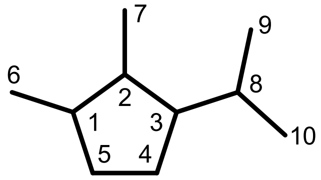


where E + is an electrophile and Z is a substituent (other than hydrogen).
See also: cine-substitution, tele-substitution

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1128

iridoids

Cyclic monoterpenoids having the iridane skeleton (1-isopropyl-2,3-di-methylcyclopentane), the traditional, but not undisputed, numbering of which is shown in the diagram.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

iron-sulfur cluster

A unit comprising two or more iron atoms and bridging sulfur ligands in an iron-sulfur protein. The recommended designation of a cluster consists of the iron and sulfur content, in square brackets, for example, [2Fe-2S], [3Fe-4S]. The possible oxidation levels are indicated by the net charge excluding the ligands, for example $[4Fe\text{-}4S]^{2+}$; $[4Fe\text{-}4S]^{+}$ or ($[4Fe\text{-}4S]^{2+;1+}$) cluster

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1281

iron-sulfur proteins

Proteins in which non-haem iron is coordinated with cysteine sulfur and usually also with inorganic sulfur. Divided into three major categories: rubredoxins; 'simple iron-sulfur proteins', containing only iron-sulfur clusters; and 'complex iron-sulfur proteins', containing additional active redox centres such as flavin, molybdenum or haem. In most iron-sulfur proteins, the clusters function as electron-transfer groups, but in others they have other functions, such as catalysis of hydratase/dehydratase reactions, maintenance of protein structure, or regulation of activity.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1281

irradiance (at a point of a surface), E

Radiant power, P, of all wavelengths incident from all upward directions on a small element of surface containing the point under consideration divided by the area of the element. SI unit is $\mathrm{W\ m^{-2}}$.
Notes:

1. Mathematical definition: $E = \frac{\mathrm{d}P}{\mathrm{d}S}$. If the radiant power is constant over the surface area considered, $E = \frac{P}{S}$.
2. Alternative definition: Integral, taken over the hemisphere visible from the given point, of the expression $L \cos\theta\, \mathrm{d}\Omega$, where L is the *radiance* at the given point in the various directions of the incident elementary beams of solid angle Ω and θ is the angle between any of the beams and the normal to the surface at the given point.

$$E = \int_{2\pi} L \cos\theta \mathrm{d}\Omega$$

3. This term refers to a beam not scattered or reflected by the target or its surroundings. For a beam incident from all directions, *fluence rate* (E_o) is an equivalent term.
4. $E = \int_{\lambda} E_{\lambda} \mathrm{d}\lambda$ where E_{λ} is the *spectral irradiance* at wavelength λ.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 357

irradiation

Exposure to ionizing radiation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

irregular macromolecule

A macromolecule the structure of which essentially comprises the repetition of more than one type of constitutional unit or a macromolecule the structure of which comprises constitutional units not all connected identically with respect to directional sense.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2289

irregular polymer

A polymer composed of irregular macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2302

irreversible transition

A transition that changes the state of a system which cannot be readily reversed to restore the system to its original state. Example: The conversion of TiO_2 (anatase) to TiO_2 (rutile).

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 584

ISC

Frequently used acronym for intersystem crossing.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 358

isoabsorption point [obsolete]

The use of this term, equivalent to isosbestic point, is not recommended.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2249

isobar

in atmospheric chemistry

Lines on a plot joining points of equal barometric pressure in the atmosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2198

isobaric mass-change determination

A technique in which the equilibrium mass of a substance at constant partial pressure of the volatile product(s) is measured as a function of temperature while the substance is subjected to a controlled temperature program. The record is the isobaric mass-change curve. The mass should be plotted on the ordinate decreasing downwards and temperature on the abscissa increasing from left to right.

Source:
Orange Book, p. 41

isobaric separation

Chromatographic separation carried out using constant inlet and outlet pressure conditions.

Source:
PAC, 1993, *65*, 2397 *(Nomenclature for supercritical fluid chromatography and extraction (IUPAC Recommendations 1993))* on page 2401

isobars

Different nuclides of equal mass number.

Source:
Physical Chemistry Division, unpublished

isoclined structures

in polymers

See: isomorphous structures *in polymers*

Source:
Purple Book, p. 43

isoclinic point

A wavelength, wavenumber, or frequency at which the first derivative of an absorption spectrum of a sample does not change upon a chemical reaction or physical change of the sample.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2249

isoconfertic separation **[obsolete]**

See: isopycnic separation

Source:
PAC, 1993, *65*, 2397 *(Nomenclature for supercritical fluid chromatography and extraction (IUPAC Recommendations 1993))* on page 2401

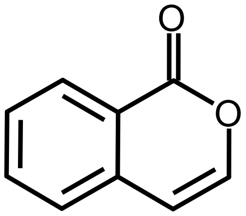
isoconjugate systems

Molecular entities with similar conjugate networks which have the same number of π-electrons, *e.g.* cyclopentadienide anion and pyrrole or benzene and pyridine.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1947

isocoumarins

Isocoumarin (1*H*-isochromen-1-one) and its derivatives formed by substitution.



See: coumarins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

isocratic analysis

in chromatography

A procedure in which the composition of the mobile phase remains constant during the elution process.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 826

isocyanates

The isocyanic acid tautomer, HN=C=O, of cyanic acid, HOC≡N and its hydrocarbyl derivatives RN=C=O.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

isocyanides

The isomer $HN^+{\equiv}C^-$ of hydrocyanic acid, HC≡N, and its hydrocarbyl derivatives RNC ($RN^+{\equiv}C^-$).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

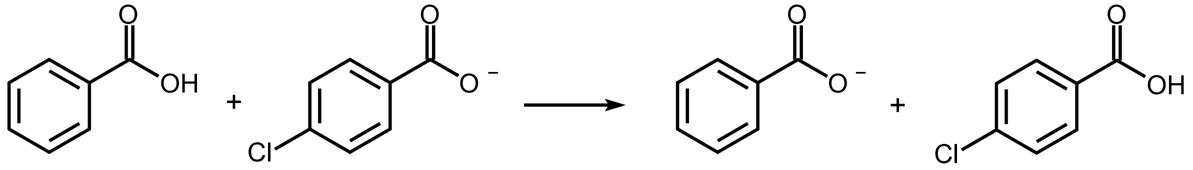
isocyclic compounds

A less preferred synonym for homocyclic compounds.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

isodesmic reaction

A reaction (actual or hypothetical) in which the types of bonds that are made in forming the products are the same as those which are broken in the reactants, e.g.

a) 

b) 

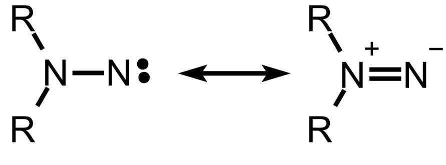
$$\mathrm{ClCH{=}CH_2 + ClCH_2{-}CH_2Cl \longrightarrow CH_2{=}CH_2 + Cl_2CH{-}CH_2Cl}$$

Such processes have advantages for theoretical treatment. The Hammett equation as applied to equilibria [cf. (a)] essentially deals with isodesmic processes.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1128

isodiazenes

Synonym: azamines

Compounds having the structure  . These compounds can also be called diazanylidenes or hydrazinylidenes. They have also been called by the trivial name azamines and the incorrectly formed name 1,1-diazenes. They should not be called aminonitrenes.
See: carbenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1344

isoelectric

A macro-ion of a polyampholyte (in particular a protein) is said to be isoelectric if it exhibits no electrophoresis.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 618

isoelectric point

in electrophoresis

The pH value at which the net electric charge of an elementary entity is zero. pI is a commonly used symbol for this kind-of-quantity. It should be replaced by pH(I) because it is a pH determined under that particular condition.

Source:
PAC, 1994, *66*, 891 *(Quantities and units for electrophoresis in the clinical laboratory (IUPAC Recommendations 1994))* on page 894
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 618

isoelectronic

Two or more molecular entities are described as isoelectronic if they have the same number of valence electrons and the same structure, i.e. number and connectivity of atoms, but differ in some of the elements involved. Thus: CO, N_2 and NO^+ are isoelectronic. $CH_2=C=O$ and $CH_2=N=N$ are isoelectronic. CH_3COCH_3 and $CH_3N=NCH_3$ have the same number of electrons, but have different structures, hence they are not described as isoelectronic.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1128

isoemissive point

Wavelength, wavenumber or frequency at which the total intensity of emission of light by a sample does not change during a chemical reaction or physical change. The terms isolampsic and isostilbic are sometimes used.
Note:
This term may be misleading because it does not specifically refer to light emission.

isoentropic

A reaction series is said to be isoentropic if the individual reactions of the series have the same standard entropy of activation.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1128

isoenzyme

One of a group of related enzymes catalysing the same reaction but having different molecular structures and characterized by varying physical, biochemical and immunological properties.

Source:
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2594
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

See also:
White Book, p. 93

isoequilibrium relationship

A relationship analogous to the isokinetic relationship but applied to equilibrium data. The equation defining the isoequilibrium temperature β is:

$$\Delta_r H - \beta\,\Delta_r S = \text{constant}$$

where ΔH and ΔS are enthalpy and entropy of reaction, respectively.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1128

isogyric reaction

A reaction in which the number of electron pairs is conserved, for example:
$CH_4(^1A_1) + H(^2S) \longrightarrow CH_3(^2A'_2) + H_2(^1\Sigma^+{}_g)$

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1947

isoionic

A macro-ion of a polyampholyte (in particular a protein) is said to be isoionic if besides the polyampholyte and H^+ or OH^- ions (in general ions of the solvent) no other ions are present in the system.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 618

isoionic point

in electrophoresis

The pH value at which the net electric charge of an elementary entity in pure water equals zero.

Source:
PAC, 1994, *66*, 891 *(Quantities and units for electrophoresis in the clinical laboratory (IUPAC Recommendations 1994))* on page 895

isokinetic line

in atmospheric chemistry

A line in a given surface connecting points with equal wind speed; also called isotach or isovel.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2198

isokinetic relationship

When a series of structurally related substrates undergo the same general reaction or when the reaction conditions for a single substrate are changed in a systematic way, the enthalpies and entropies of activation sometimes satisfy the relation:

$$\Delta^{\ddagger}H - \beta\,\Delta^{\ddagger}S = \text{constant}$$

where the parameter β is independent of temperature. This equation (or some equivalent form) is said to represent an 'isokinetic relationship'. The temperature $T = \beta$ (at which all members of a series obeying the isokinetic relationship react at the same rate) is termed the 'isokinetic temperature'. Supposed isokinetic relationships as established by direct correlation of $\Delta^{\ddagger}H$ with $\Delta^{\ddagger}S$ are often spurious and the calculated value of β is meaningless, because errors in $\Delta^{\ddagger}H$ lead to compensating errors in $\Delta^{\ddagger}S$. Satisfactory methods of establishing such relationships have been devised.
See also: compensation effect, isoequilibrium relationship, isoselective relationship

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1129

isokinetic sampling

in atmospheric chemistry

A technique for collecting airborne particulate in which the sampling device has a collection efficiency of unity for all sizes of particles in sampled air, regardless of wind velocity and direction of the instrument. The air stream entering the collector has a velocity (speed and direction) equal to that of the air in the gas stream just ahead of the sampling port of the collector.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2198

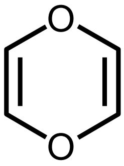
isolampsic point

Same as isoemissive point.
Note:
The term derives from the Greek words isos: equal, and lampein: to emit light or to shine. Isolampsic is thus parallel to isosbestic.

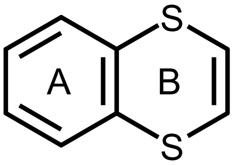
Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 358

isolated double bonds

Those bonds which are neither conjugated nor cumulative as in



or the B ring of



Source:
Blue Book, p. 69

isolobal

The term is used to compare molecular fragments with each other and with familiar species from organic chemistry. Two fragments are isolobal if the number, symmetry properties, approximate energy and shape of the frontier orbitals and the number of electrons in them are similar.
See: isoelectronic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1129

isomer

One of several species (or molecular entities) that have the same atomic composition (molecular formula) but different line formulae or different stereochemical formulae and hence different physical and/or chemical properties.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1129
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

isomer shift

in Mössbauer spectroscopy

Measure of the energy difference between the source (E_s) and the absorber (E_a) transition. The measured Doppler velocity shift, δ, is related to the energy difference by

$$E_a - E_s = \frac{\delta\, E_\gamma}{c}$$

where E_γ is the Mössbauer gamma energy and c is the speed of light in vacuum.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 214

isomerases

Enzymes that catalyse intramolecular rearrangements. Isomerases are classified into racemases and epimerases, *cis-trans* isomerases, intramolecular lyases and other isomerases.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

isomeric

Adjective derived from isomer.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

isomeric state

in nuclear chemistry

A nuclear state having a mean life long enough to be observed.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1545

isomeric transition

in nuclear chemistry

A spontaneous transition between two isomeric states of a nucleus.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1545

isomerism

The relationship between isomers.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

isomerization

A chemical reaction, the principal product of which is isomeric with the principal reactant. An intramolecular isomerization that involves the breaking or making of bonds is a special case of a molecular rearrangement. Isomerization does not necessarily imply molecular rearrangement (e.g. in the case of the interconversion of conformational isomers).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1129

isometric

Also contains definition of: anisometric

Two molecular entities that are superposable or can be made superposable by reflection of one of them in a mirror are isometric; otherwise they are anisometric.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2210

isomorphic polymer blend

Polymer blend of two or more different semi-crystalline polymers that are miscible in the crystalline state as well as in the molten state.
Notes:

1. Such a blend exhibits a single, composition-dependent glass-transition temperature, T_g, and a single, composition-dependent melting point, T_m.
2. This behaviour is extremely rare; very few cases are known.

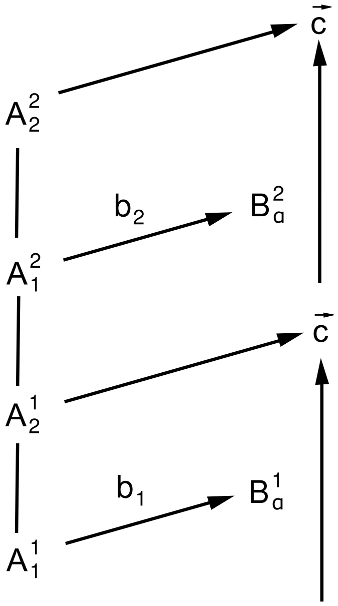
Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1988

isomorphous structures

Also contains definition of: enantiomorphous structures *in polymers*

in polymers

In the crystalline state, polymer chains are generally parallel to one another but neighbouring chains of equivalent conformation may differ in chirality and/or orientation. Chains of identical chirality and conformation are isomorphous. Chains of opposite chirality but equivalent conformation are enantiomorphous. For example, two ...$TG^+TG^+TG^+$... helices of isotactic poly(propylene) are isomorphous. Isotactic poly(propylene) chains of the ...$TG^+TG^+TG^+$... and ...$G^-TG^-TG^-T$... types are mutually enantiomorphous. With regard to orientation, consider a repeating side group originating at atom A_1^i, the first atom of the side group being B_α^i. For certain chain symmetries (helical, for instance) the bond vectors $\vec{\mathbf{b}}(A_1^i, B_\alpha^i)$ have the same components (positive or negative) $\frac{\vec{\mathbf{b}} \cdot \vec{\mathbf{c}}}{|\vec{\mathbf{c}}|}$ along the c axis for every i.



Two equivalent (isomorphous or enantiomorphous) chains in the crystal lattice, having identical components of the bond vectors along c, both positive or both negative, are designated isoclined; two equivalent chains having bond vectors along c of the same magnitude but opposite sign are designated anticlined.

Source:
Purple Book, p. 43

isonitriles [obsolete]

An obsolete term, which should not be used, for isocyanides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

isonitroso compounds [obsolete]

An obsolete term for oximes, based on the fact that compounds with a nitroso group, –N=O, bonded to a $–CR_2H$ group readily tautomerize to oximes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

isooptoacoustic point

Wavelength, wavenumber or frequency at which the total energy emitted by a sample as heat does not change upon a chemical reaction in or a physical change of the sample. Its position depends on the experimental conditions.
Note:
The spectral differences between the isosbestic points and the iso-optoacoustic points are the result of the non-linear relationship between the molar absorption coefficient and the photoacoustic signal.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 358

isopeptide bond

See: peptides

Source:
White Book, p. 48

isopotential point

For an ion-selective electrode cell, there is often a particular activity of the measured ion for which the emf of the cell is independent of temperature. That activity, and the corresponding potential difference, defines the isopotential point. The specification of the ion-selective electrode and outer reference electrode must be described. Comment: When an isothermal cell is used with identical reference electrodes, the isopotential point is the activity of sensed species that gives zero net membrane potential, e.g. sensed activity is the same in the inner and outer (test) solution. Calibration lines for different cell temperatures have different slopes, but intersect at a common activity point. Cells with temperature gradients are not recommended.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2531

isoprenes

See: prenols

Source:
White Book, p. 252

isoprenoids

Compounds formally derived from isoprene (2-methylbuta-1,3-diene), the skeleton of which can generally be discerned in repeated occurrence in the molecule. The skeleton of isoprenoids may differ from strict additivity of isoprene units by loss or shift of a fragment, commonly a methyl group. The class includes both hydrocarbons and oxygenated derivatives.
See also: carotenoids, steroids, terpenes, terpenoids, prenols

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

See also:
White Book, p. 255

isopycnic

An adjective describing components of a multicomponent system with equal partial specific volumes.

Source:
Purple Book, p. 60

isopycnic separation

Chromatographic separations carried out using constant density conditions. The temperature and pressure may be altered during the run (originally the term isoconfertic separation was used but this term is not recommended).

Source:
PAC, 1993, *65*, 2397 *(Nomenclature for supercritical fluid chromatography and extraction (IUPAC Recommendations 1993))* on page 2401

isorefractive

An adjective describing components of a multicomponent system having zero refractive index increments with respect to each other.

Source:
Purple Book, p. 68

isosbestic point

Wavelength, wavenumber or frequency at which the total absorbance of a sample does not change during a chemical reaction or a physical change of the sample.
Notes:

1. A simple example occurs when one molecular entity is converted into another that has the same molar absorption coefficient at a given wavelength. As long as the sum of the concentrations of the two molecular entities in the solution is held constant there will be no change in absorbance at this wavelength as the ratio of the concentrations of the two entities is varied.
2. The name derives from the Greek words: isos: equal, the same, and sbestos: extinguishable.
3. Contrary to a widely accepted idea, the existence of an isosbestic point does not prove that the reaction is a quantitative conversion of one species into a unique other species or that an equilibrium exists between only two species. The observation of isosbestic points only indicates that the stoichiometry of the reaction remains unchanged during the chemical reaction or the physical change of the sample, and that no secondary reactions occur during the considered time range, since $A_\lambda\, l^{-1} = \sum_{i=1}^{n} \varepsilon_i(\lambda)\, c_i$ is invariant (A_λ is the absorbance at wavelength λ, l is the optical path, ε_i is the molar decadic absorption coefficient of the species i of concentration c_i). For the reaction A + B → *c* C + *d* D + *e* E, with *c*, *d*, and *e* the percentages of the products C, D, and E, an isosbestic point will be observed at every wavelength where the condition $\varepsilon_\mathrm{A} + \varepsilon_\mathrm{B} = c\,\varepsilon_\mathrm{C} + d\,\varepsilon_\mathrm{D} + e\,\varepsilon_\mathrm{E}$, provided that the values of the percentages *c*, *d*, and *e* remain constant during the chemical reaction or the physical change. The use of the obsolete term isoabsorption point is not recommended.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 359

isoselective relationship

A relationship analogous to the isokinetic relationship, but applied to selectivity data of reactions. At the isoselective temperature, the selectivities of the series of reactions following the relationship are identical.
See also: isoequilibrium relationship

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1130

isoselenocyanates

Selenium analogues of isocyanates RN=C=Se.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

isostatic pressing

Application of a hydrostatic pressure through a liquid to achieve densification prior to the production of a uniform compact monolith through ceramization of the densified liquid.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1824

isosteric enthalpy of adsorption

When the addition of the differential amount of component i $\mathrm{d}n_i^{\sigma}$ or $\mathrm{d}n_i^{\mathrm{s}}$ is effected at constant pressure p, the differential molar enthalpy of adsorption, $\Delta_a H_i^{\sigma}$ or $\Delta_a H_i^{\mathrm{s}}$ also called the isosteric enthalpy of adsorption (q^{st}) is defined as:

$$\Delta_a H_i^{\sigma} = -q^{\mathrm{st},\sigma} = U_i^{\sigma} - H_i^{\mathrm{g}}$$

$$\Delta_a H_i^{\mathrm{s}} = -q^{\mathrm{st},\sigma} = H_i^{\sigma} - H_i^{\mathrm{g}}$$

where $H_i^{\mathrm{s}} = \left(\frac{\partial H^{\mathrm{s}}}{\partial n_i^{\mathrm{s}}}\right)_{T,p,m,n_j^{\mathrm{s}}}$ and H_i^{g} is the partial molar enthalpy of component i in the gas phase, i.e. $\left(\frac{\partial H^{\mathrm{g}}}{\partial n_i^{\mathrm{g}}}\right)_{T,p,n_i^{\mathrm{g}}}$

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 603

isostilbic point

Same as isoemissive point.
Note:
From the Greek words: isos: equal, and stilbein: to shine.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 359

isostructural reaction

A ligand exchange reaction, where the structural type of the metal complex remains the same.
$ML_n + X \longrightarrow ML_{n-1}X + L + \Delta E$

Although these types of reactions are not necessarily isodesmic reactions, a substantial degree of error cancellation for the calculated energy, ΔE, is achieved because the coordination sphere of the metal atom M is conserved.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1948

isotactic macromolecule

A tactic macromolecule, essentially comprising only one species of configurational base unit, which has chiral or prochiral atoms in the main chain in a unique arrangement with respect to its adjacent constitutional units.
Notes:
1. In an isotactic macromolecule, the configurational repeating unit is identical with the configurational base unit.
2. An isotactic macromolecule consists of meso diads.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2292

isotactic polymer

A polymer composed of isotactic macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2302

isotactic triads

in polymers

See: triads

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2299

isotherm

in atmospheric chemistry

Lines joining points of equal temperature in the atmosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2198

isothermal chromatography

A procedure in which the temperature of the column is kept constant during the separation.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 827

isothiocyanates

Sulfur analogues of isocyanates RN=C=S.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

isotones

Nuclides having the same neutron number but different atomic numbers.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1545

isotope dilution

Mixing of a given nuclide with one or more of its isotopes.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

isotope dilution analysis

A kind of quantitative analysis based on the measurement of the isotopic abundance of a nuclide after isotope dilution with the test portion.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

isotope effect

Also contains definition of: equilibrium isotope effect

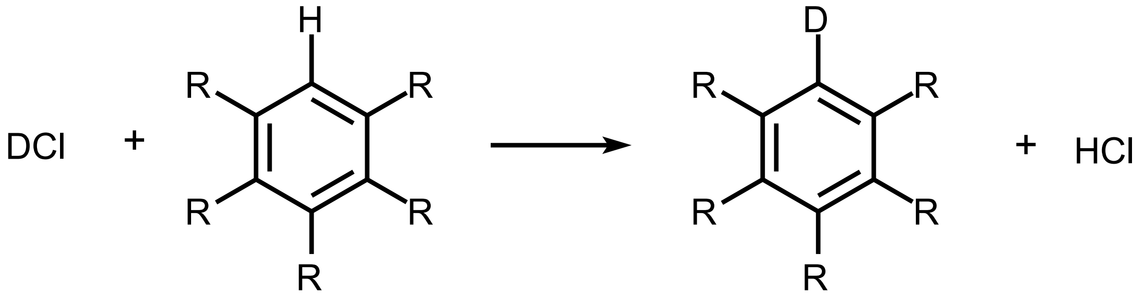
The effect on the rate or equilibrium constant of two reactions that differ only in the isotopic composition of one or more of their otherwise chemically identical components is referred to as a kinetic isotope effect or a thermodynamic (or equilibrium) isotope effect, respectively.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1130
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 170

isotope exchange

A chemical reaction in which the reactant and product chemical species are chemically identical but have different isotopic composition. In such a reaction the isotope distribution tends towards equilibrium (as expressed by fractionation factors) as a result of transfers of isotopically different atoms or groups. For example:



Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1132
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

isotope exchange analysis

A kind of quantitative analysis based on the isotope exchange between isotopes of the element to be determined and other isotopes of this element in different valency states or in different molecules.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

isotope pattern

in mass spectrometry

Set of peaks related to ions with the same chemical formula but containing different isotopes; e.g. the 16 and 17 mass/charge peaks in a CH_4 sample arising from $^{12}CH_4^+$ and $^{13}CH_4^+$ ions

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2198

isotopes

Nuclides having the same atomic number but different mass numbers.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520
Red Book, p. 35

See also:
Orange Book, p. 230

isotopic abundance

The relative number of atoms of a particular isotope in a mixture of the isotopes of an element, expressed as a fraction of all the atoms of the element.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

isotopic carrier

A carrier which differs only in isotopic composition from the trace it has to carry.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

isotopic enrichment

Any process by which the isotopic abundance of a specified isotope in a mixture of isotopes of an element is increased.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

isotopic enrichment factor

For a material enriched in a specified isotope, the ratio between the isotopic abundance and the natural abundance of that isotope.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

isotopic fractionation factor

The ratio

$$\frac{(x_1/x_2)_{\mathrm{A}}}{(x_1/x_2)_{\mathrm{B}}},$$

where x is the abundance, expressed as the atom fraction of the isotope distinguished by the subscript numeral, when the two isotopes are equilibrated between two different chemical species A and B (or between specific sites **A** and **B** in the same or different chemical species). The term is most commonly met in connection with deuterium solvent isotope effects, when the fractionation factor Φ expresses the ratio:

$$\Phi = \frac{(x_{\mathrm{D}}/x_{\mathrm{H}})_{\mathrm{solute}}}{(x_{\mathrm{D}}/x_{\mathrm{H}})_{\mathrm{solvent}}}$$

for the exchangeable hydrogen atoms in the chemical species (or sites) concerned. The concept is also applicable to transition states.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1115

isotopic ion

Any ion containing one or more of the less abundant naturally occurring isotopes of the elements that make up its structure, e.g. CH_2D^+ .

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549
Orange Book, p. 205

isotopic labelling

Labelling in which the resulting product is only different from the initial one by its isotopic composition.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

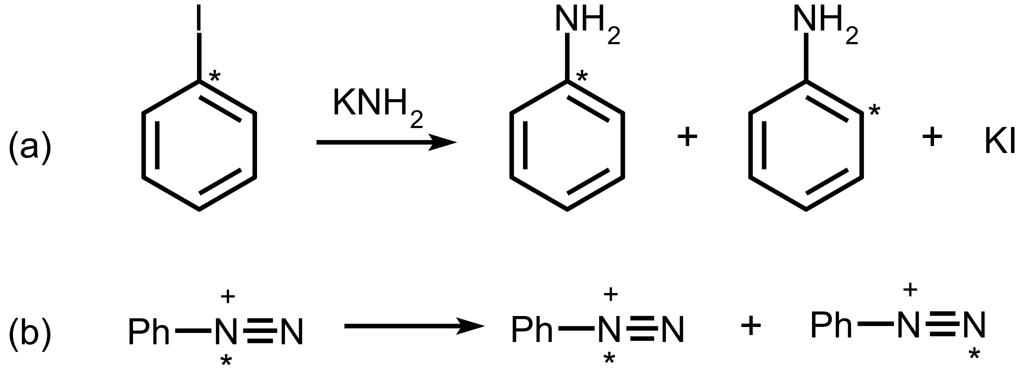
isotopic molecular ion

A molecular ion containing one or more of the less abundant naturally occurring isotopes of the atoms that make up the molecular structure. Thus, for ethyl bromide there exist isotopic molecular ions such as: $^{13}CCH_5Br^{+\cdot}$, $C_2H_4DBr^{+\cdot}$, $C_2H_5{}^{81}Br^{+\cdot}$, $^{13}C_2H_5{}^{81}Br^{+\cdot}$, etc.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

isotopic scrambling

The achievement, or the process of achieving, an equilibrium distribution of isotopes within a specified set of atoms in a chemical species or group of chemical species (for an example, see diagram).



See also: fractionation factor

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1132

See also:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1556

isotopic separation

An operation for the purpose of modifying an isotopic abundance in a mixture of isotopes.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1545

isotopic tracer

A tracer which only differs in isotopic composition from the substance to be traced.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

isotopically deficient

An isotopically labelled compound may be designated as isotopically deficient when the isotopic content of one or more elements has been depleted, i.e. when one or more nuclide(s) is (are) present in less than a natural ratio.

Source:
Blue Book, p. 518
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1896

isotopically enriched ions

When the abundance of a particular nuclide is increased above the level at which it occurs in nature and is incorporated in a molecule, the term 'isotopically enriched ion' is used to describe any ion enriched in the isotope.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

isotopically labelled

Describes a mixture of an isotopically unmodified compound with one or more analogous isotopically substituted compound(s).

Source:
Blue Book, p. 514
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1891

isotopically modified

Describes a compound that has a macroscopic composition such that the isotopic ratio of nuclides for at least one element deviates measurably from that occurring in nature. It is either an isotopically substituted compound or an isotopically labelled compound.

Source:
Blue Book, p. 514
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1889

isotopically substituted

Describes a compound that has a composition such that essentially all the molecules of the compound have only the indicated nuclide(s) at each designated position. For all other positions, the absence of nuclide indication means that the nuclide composition is the natural one.

Source:
Blue Book, p. 514
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1890

isotopically unmodified

Describes a compound that has a macroscopic composition such that its constituent nuclides are present in the proportions occurring in nature.

Source:
Blue Book, p. 514
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1889

isotopologue

A molecular entity that differs only in isotopic composition (number of isotopic substitutions), e.g. CH_4, CH_3D, CH_2D_2.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1132

isotopomer

Isomers having the same number of each isotopic atom but differing in their positions. The term is a contraction of 'isotopic isomer'. Isotopomers can be either constitutional isomers (e.g. $CH_2DCH{=}O$ and $CH_3CD{=}O$) or isotopic stereoisomers [e.g. (*R*)- and (*S*)-CH_3CHDOH or (*Z*)- and (*E*)-$CH_3CH{=}CHD$].

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1132
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2211

isotropic

A quantity which is independent of direction. Anisotropic and nonisotropic refer to quantities which are direction dependent.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2198

isotropic carbon

A monolithic carbon material without preferred crystallographic orientation of the microstructure.
Note:
Isotropic carbon can also be a graphite material. The isotropy can be gross (bulk), macroscopic or microscopic, depending on the structural level at which isotropy is obtained. This word is widely used today and its meaning covers all the above levels. For example, the aerospace graphites have isotropy built in by random grain orientation. Some nuclear graphites are isotropic at the crystalline (sub-grain) level.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 495

isotropic pitch-based carbon fibres

Carbon fibres obtained by carbonization of isotropic pitch fibres after these have been stabilized (i.e. made non-fusible).
Note:
During fabrication of isotropic pitch-based carbon fibres no means (neither mechanical nor chemical) are applied to achieve preferred orientation of the polyaromatic molecules in the fibre direction. They belong to the carbon fibres type LM (low modulus), and because of the relatively low values of strength and Young's modulus this pitch-based carbon fibre type is not used for high-performance reinforcement purposes.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 495

isoureas

The imidic acid tautomer of urea, $H_2NC(=NH)OH$, and its hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

isozyme

Synonymous with isoenzyme.

Source:
White Book, p. 93

j-value

in atmospheric chemistry

An effective first order rate constant for a photochemical reaction (photodecomposition, etc.) of light-absorbing impurities in the atmosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2198

Jablonski diagram

Originally, a diagram showing that the fluorescent state of a molecular entity is the lowest excited state from which the transition to the ground state is allowed, whereas the phosphorescent state is a metastable state below the fluorescent state, which is reached by radiationless transition. In the most typical cases the fluorescent state is the lowest singlet excited state and the phosphorescent state the lowest triplet state, the ground state being a singlet. Presently, modified Jablonski diagrams are frequently used and are actually state diagrams in which molecular electronic states, represented by horizontal lines displaced vertically to indicate relative energies, are grouped according to multiplicity into horizontally displaced columns. Excitation and relaxation processes that interconvert states are indicated in the diagram by arrows. Radiative transitions are generally indicated with straight arrows (→), while radiationless transitions are generally indicated with wavy arrows ⇝.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2250

Jahn–Teller effect

Molecular distortions due to an electronically degenerate ground state. For non-linear molecular entities in a geometry described by a point symmetry group possessing degenerate irreducible representations there always exists at least one non-totally symmetric vibration that makes electronically degenerate states unstable at this geometry. The nuclei are displaced to new equilibrium positions of lower symmetry causing a splitting of the originally degenerate states (first-order Jahn–Teller effect).
Note:
Effect due to the odd terms in the vibronic perturbation expansion. In the case of molecules with a non-degenerate ground electronic state but with a low-lying degenerate excited state, distortions of proper symmetry arise that result in mixing of the ground and excited states, thereby lowering the ground-state energy (pseudo Jahn–Teller effect). The pseudo Jahn–Teller effect manifests itself in fluxional behaviour (see fluxional molecules) and stereochemical non-rigidity of molecules and ions. The Jahn–Teller effect generates a surface crossing (e.g., a conical intersection) whereas a pseudo Jahn–Teller effect generates an avoided crossing.
See also: Renner–Teller effect

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 360

Jahn–Teller transition

A displacive crystal distortion to lower symmetry that cooperatively removes a localized-electron orbital degeneracy at an array of like atoms so as to leave the atoms in the centre of symmetry of their distorted sites. Example: The crystallographic distortion in Mn_3O_4.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 584

joule

SI derived unit of energy, $\mathrm{J = N\,m = kg\,m^2\,s^{-2}}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 977

junction point

Branch point in a polymer network.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1819

junction unit

A non-repeating atom or non-repeating group of atoms between blocks in a block macromolecule.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2293

junction-point density

Number of junction points per unit volume in a polymer network.
See also: crosslink density

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1820

κ (kappa)

in inorganic nomenclature

An affix in the name of a polydentate chelate complex indicating single ligating atom attachments of a polyatomic ligand to a coordination centre. A right superscript numerical index indicates the number of such attachments. Example: $Ni[(CH_3)_2PCH_2CH_2P(CH_3)_2]Br_2$, dibromobis[1,2-ethanediylbis(dimethylphosphine)-$\kappa^2 P$]nickel(II).

Source:
Red Book, p. 174

Kamlet–Taft solvent parameters

Parameters of the Kamlet–Taft solvatochromic relationship which measure separately the hydrogen bond donor (α), hydrogen bond acceptor (β), and dipolarity/polarizability (π*) properties of solvents as contributing to overall solvent polarity.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1132

Kaptein–Closs rules

Rules used to predict the sign of CIDNP effects.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2250

Kasha rule

Polyatomic molecular entities luminesce with appreciable yield only from the lowest excited state of a given multiplicity. There are exceptions to this rule.
Note:
The concept has been extended to the reaction of excited species, i.e., polyatomic molecular entities react with appreciable yield only from the lowest excited state of a given multiplicity.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 360

Kasha–Vavilov rule

The quantum yield of luminescence is independent of the wavelength of exciting radiation. There are exceptions to this rule.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2250

katal

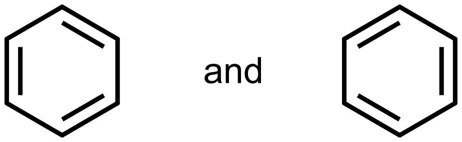
Unit for catalytic activity coherent with the SI, equal to the catalytic activity that catalyses a reaction rate of one mole per second in an assay system. $1\ \text{kat} = 1\ \text{mol s}^{-1}$. The katal is recommended for use in the specific context of enzymes and clinical chemistry.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 977

See also:
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2595

Kekulé structure (for aromatic compounds)

A representation of an aromatic molecular entity (such as benzene), with fixed alternating single and double bonds, in which interactions between multiple bonds are assumed to be absent. For benzene:



are the Kekulé structures.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1132

kelvin

SI base unit of thermodynamic temperature (symbol: K). The kelvin is the fraction 1/273.16 of the thermodynamic temperature of the triple point of water.

Source:
Green Book, 2nd ed., p. 70
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 977

ketals

Acetals derived from ketones by replacement of the oxo group by two hydrocarbyloxy groups $R_2C(OR)_2$ ($R \neq H$). This term, once abandoned, has been reinstated as a subclass of acetals.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

ketazines

Azines of ketones $R_2C{=}NN{=}CR_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

ketenes

Compounds in which a carbonyl group is connected by a double bond to an alkylidene group $R_2C{=}C{=}O$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

ketenimines

Compounds having the structure $R_2C{=}C{=}NR$. Thus imino analogues of ketenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

ketimines

Compounds having the structure $R_2C{=}NR'$ ($R \neq H$).
See: imines

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

keto

See: oxo compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

keto carbenes

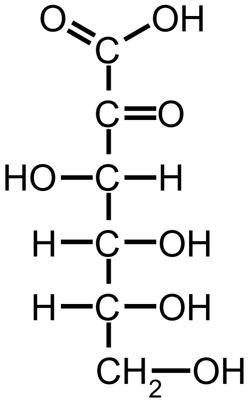
The term has imprecisely been used to designate carboxylic acyl carbenes. Keto carbenes are carbenes bearing an oxo function at an unspecified site.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1345

ketoaldonic acids

Also contains definition of: ulosonic acids

Monosaccharides in which a structure containing a keto group and a carboxylic acid group is in equilibrium with a hemiacetal structure. Specific compounds are named using the -ulosonic acid suffix. E.g. D-*arabino*-hexulosonic acid:



See also: oxo compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1346

ketoaldoses

Monosaccharides which contain both an aldehydic and a ketonic carbonyl group in equilibrium with intramolecular hemiacetal forms.
See also: oxo compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1346

ketones

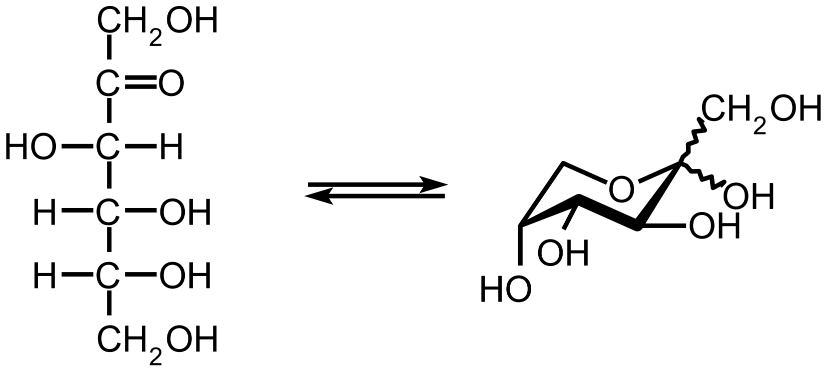
Compounds in which a carbonyl group is bonded to two carbon atoms $R_2C=O$ (neither R may be H).
Note:

Compounds of structure such as $R_3SiC(=O)R$ are not ketones but acyl derivatives of substituted silanes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1346

ketoses

Ketonic parent sugars (polyhydroxyketones $H–[CHOH]_n–C(=O)[CHOH]_m–H$ with three or more carbon atoms) and their intramolecular hemiacetals. The oxo group is usually at C-2. E.g. D-fructose:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1346
White Book, p. 129

ketoximes

Oximes of ketones, $R_2C=NOH$ ($R \neq H$).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1346

ketyls

Radical anions (or the corresponding salts) derived from ketones by addition of an electron $R_2C^{\cdot}–O^{-} \longleftrightarrow R_2C^{-}–O^{\cdot}$.
Note:
Ketyls produce two types of conjugate acids: $R_2C^{\cdot}–OH$ and $R_2CH–O^{\cdot}$. The former are α-hydroxyalkyl radicals and the latter are alkoxyl radicals, but they have also been called ketyls in photochemistry.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1346

kilo

SI prefix for 10^3 (symbol: k).

Source:
Green Book, 2nd ed., p. 74

kilogram

SI base unit for mass (symbol: kg). The kilogram is equal to the mass of the international prototype of the kilogram.

Source:
Green Book, 2nd ed., p. 70
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 978

kind-of-property

An attribute of phenomena, bodies or substances that may be distinguished qualitatively. Examples: Colour (value: green, blue), transparency, length (value: long, short; $2\ \mathrm{m}, 5\ \mathrm{m}$), amount-of-substance (value: $2\ \mathrm{mol}, 5\ \mathrm{mol}$). Kind-of-property includes the concept kind-of-quantity. All kinds-of-property may be related to nominal (e.g. green, blue) and ordinal scales (e.g. small, large), but kinds-of-quantity are generally related to difference [e.g. $10\ °\mathrm{C}$ (i.e. $10\ °\mathrm{C}$ more than an arbitrary zero)] or ratio scales (length $2\ \mathrm{m}$ or $5\ \mathrm{m}$).

Source:
PAC, 1995, *67*, 1563 *(Properties and units in the clinical laboratory sciences-I. Syntax and semantic rules (IUPAC-IFCC Recommendations 1995))* on page 1565

kind-of-quantity

Abstract property common to several real quantities.
See: quantity

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 978

kinematic viscosity, ν

Dynamic viscosity divided by the density of the fluid.

Source:
Green Book, 2nd ed., p. 13
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 978

kinematics

The study of the properties of motion that are independent of the nature of the forces. In reaction dynamics the term is often applied in particular to effects that occur when atomic masses are changed, the forces remaining the same.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 170

kinetic activity factor

A factor involving activity coefficients that appears as a multiplier in the rate equation. For a bimolecular reaction the factor is

$$\frac{y_{\mathrm{A}}\, y_{\mathrm{B}}}{y_{\ddagger}},$$

where y_{A}, y_{B} and $y_{\ddagger}$ are the activity coefficients for the reactants A and B and the activated complex, respectively. For a unimolecular reaction the factor is

$$\frac{y_{\mathrm{A}}}{y_{\ddagger}},$$

and for a trimolecular reaction it is

$$\frac{y_{\mathrm{A}}\, y_{\mathrm{B}}\, y_{\mathrm{C}}}{y_{\ddagger}}.$$

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 171

kinetic ambiguity

See: kinetic equivalence

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1133

kinetic control

of product composition

The term characterizes conditions (including reaction times) that lead to reaction products in a proportion governed by the relative rates of the parallel (forward) reactions in which the products are formed, rather than by the respective overall equilibrium constants.
See also: thermodynamic control

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1133

kinetic current

Also contains definitions of: surface reaction *in electrochemistry*, volume reaction *in electrochemistry*

A faradaic current that corresponds to the reduction or oxidation of an electroactive substance formed by a prior chemical reaction from another substance that is not electroactive, and that is partially or entirely controlled by the rate of that reaction. The reaction may be heterogeneous, occurring at an electrode-solution interface (surface reaction), or it may be homogeneous, occurring at some distance from the interface (volume reaction).

Source:
Orange Book, p. 55

kinetic electrolyte effect (kinetic ionic-strength effect)

Also contains definitions of: primary kinetic electrolyte effect, secondary kinetic electrolyte effect

The general effect of an added electrolyte (i.e. an effect other than, or in addition to, that due to its possible involvement as a reactant or catalyst) on the observed rate constant of a reaction in solution. At low concentrations (when only long-range coulombic forces need to be considered) the effect on a given reaction is determined only by the ionic strength of the solution and not by the chemical identity of the ions. For practical purposes, this concentration range is roughly the same as the region of validity of the Debye–Hückel limiting law for activity coefficients. At higher concentrations, the effect of an added electrolyte depends also on the chemical identity of the ions. Such specific action can usually be interpreted as the incursion of a reaction path involving an ion of the electrolyte as reactant or catalyst, in which case the action is not properly to be regarded just as a kinetic electrolyte effect. Kinetic electrolyte effects are usually (too restrictively and therefore incorrectly) referred to as 'kinetic salt effects'. A kinetic electrolyte effect ascribable solely to the influence of the ionic strength on activity coefficients of ionic reactants and transition states is called a 'primary kinetic electrolyte effect'. A kinetic electrolyte effect arising from the influence of the ionic strength of the solution upon the pre-equilibrium concentration of an ionic species that is involved in a subsequent rate-limiting step of a reaction is called a 'secondary kinetic electrolyte effect'. A common case encountered in practice is the effect on the concentration of hydrogen ion (acting as catalyst) produced from the ionization of a weak acid in a buffer solution. Synonymous with kinetic equivalence.
See also: common-ion effect, order of reaction, kinetic ambiguity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1133

kinetic energy, E_k

Energy of motion: for a body of mass m,

$$E_k = \frac{m\,v^2}{2},$$

where v is the speed.

Source:
Green Book, 2nd ed., p. 12
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 978

kinetic equivalence

Two reaction schemes are kinetically equivalent if they imply the same rate law. For example, consider the two schemes (i) and (ii) for the formation of C from A:

$$\text{(i)}\qquad \mathrm{A} \xrightleftharpoons[k_{-1},\mathrm{OH}^-]{k_1,\mathrm{OH}^-} \mathrm{B} \overset{k_2}{\rightarrow} \mathrm{C}$$

Providing that B does not accumulate as a reaction intermediate.

$$\frac{\mathrm{d}[\mathrm{C}]}{\mathrm{d}t} = \frac{k_1\,k_2\,[\mathrm{A}]\,[\mathrm{OH}^-]}{k_2 + k_{-1}\,[\mathrm{OH}^-]}$$

$$\text{(ii)}\qquad \mathrm{A} \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} \mathrm{B} \xrightarrow[\mathrm{OH}^-]{k_2} \mathrm{C}$$

Providing that B does not accumulate as a reaction intermediate:

$$\frac{\mathrm{d}[\mathrm{C}]}{\mathrm{d}t} = \frac{k_1\,k_2\,[\mathrm{A}]\,[\mathrm{OH}^-]}{k_{-1} + k_2\,[\mathrm{OH}^-]}$$

Both equations for $\frac{\mathrm{d}[\mathrm{C}]}{\mathrm{d}t}$ are of the form:

$$\frac{\mathrm{d}[\mathrm{C}]}{\mathrm{d}t} = \frac{r\,[\mathrm{A}]\,[\mathrm{OH}^-]}{1 + s\,[\mathrm{OH}^-]}$$

where r and s are constants (sometimes called 'coefficients in the rate equation'). The equations are identical in their dependence on concentrations and do not distinguish whether OH^- catalyses the formation of B, and necessarily also its reversion to A, or is involved in its further transformation to C. The two schemes are therefore kinetically equivalent under conditions to which the stated provisos apply.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1133

kinetic isotope effect

The effect of isotopic substitution on a rate constant is referred to as a kinetic isotope effect. For example, in the reaction:

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C}$$

the effect of isotopic substitution in reactant A is expressed as the ratio of rate constants $\frac{k^{\mathrm{l}}}{k^{\mathrm{h}}}$, where the superscripts l and h represent reactions in which the molecules A contain the light and heavy isotopes, respectively. Within the framework of transition state theory in which the reaction is rewritten as:

$$\mathrm{A} + \mathrm{B} \rightleftarrows [\mathrm{TS}]^{\ddagger} \longrightarrow \mathrm{C}$$

and with neglect of isotopic mass on tunnelling and the transmission coefficient, $\frac{k^{\mathrm{l}}}{k^{\mathrm{h}}}$ can be regarded as if it were the equilibrium constant for an isotope exchange reaction between the transition state $[\mathrm{TS}]^{\ddagger}$ and the isotopically substituted reactant A, and calculated from their vibrational frequencies as in the case of a thermodynamic isotope effect. Isotope effects like the above, involving a direct or indirect comparison of the rates of reaction of isotopologues, are called 'intermolecular', in contrast to intramolecular isotope effects, in which a single substrate reacts to produce a non-statistical distribution of isotopomeric product molecules.
See also: isotope effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1130

kinetic method

of analysis

An analytical method in which the rate of a reaction or a related quantity is measured and utilized to determine concentrations.

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2296

kinetic resolution

The achievement of partial or complete resolution by virtue of unequal rates of reaction of the enantiomers in a racemate with a chiral agent (reagent, catalyst, solvent, etc.).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2211

kinetic synergist [obsolete]

This term is not recommended for catalyst or accelerator.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2381

kinetic theory of collisions

See: collision theory

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 171

klado-

An affix used in names to designate a very open polyboron structure.

Source:
Red Book, p. 245

Koopmans' theorem

Directly relates experimental ionization potentials with energy levels of molecular orbitals. The theorem states that the ionization potential required to remove an electron from the orbital Ψ_i is given by the negative value of the energy of the orbital, $-\varepsilon_i$, as calculated within the Hartree–Fock approximation. The theorem is not applied to localized molecular orbitals, which are not eigenfunctions of the effective hamiltonian.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1949

Koppel–Palm solvent parameters

Parameters to measure separately the ability of a solvent to enter into non-specific solvent–solute interactions (permittivity ε and refractive index η_D) and specific solvent–solute interaction (solvent basicity or nucleophilicity B and solvent acidity or electrophilicity E) as contributing to overall solvent polarity.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1134

Kosower *Z*-value

See: *Z*-value

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1134

Krafft point

The temperature (more precisely, narrow temperature range) above which the solubility of a surfactant rises sharply. At this temperature the solubility of the surfactant becomes equal to the critical micelle concentration. It is best determined by locating the abrupt change in slope of a graph of the logarithm of the solubility against t or $\frac{1}{T}$.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

Kratky plot

A diagrammatic representation of scattering data on large particles, obtained at different angles but at the same concentration, constructed by plotting $\left(\sin\frac{\theta}{2}\right)^2 \Delta R(\theta)$ vs. $\left(\sin\frac{\theta}{2}\right)^2$, or $q^2\ \Delta R(\theta)$ vs. q and used for the determination of molecular shape. $\Delta R(\theta)$ is the excess Rayleigh ratio, $P(\theta)$ the particle scattering function, θ the scattering angle and q the length of the scattering vector.

Source:
Purple Book, p. 67

krypton ion laser

A CW or pulsed laser emitting lines from 337 to $859\ \mathrm{nm}$ from singly ionized krypton. Principal emissions are at 530.9, 568.2, 647.1 and $752.5\ \mathrm{nm}$.
See: gas lasers

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2250

λ-transition (lambda-transition)

A second-order or higher-order transition, in which the heat capacity shows either a discontinuity (second-order) or a vertex (higher-order) at the transition temperature. Example: The transition at $846\ \mathrm{K}$, accompanied by a finite change in specific heat capacity at constant pressure C_p, of the low-temperature polymorph of quartz to the high-temperature polymorph.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 584

l, *u*

Stereodescriptors of diastereoisomers with two chirality elements. When the two chirality elements are both *R* or both *S* the molecular entity is described as having an *l* relationship (*l* = like), when one chirality element is *R* and the other *S* the molecular entity is described as having a *u* relationship (*u* = unlike). The notation can be extended to molecules with more than two chirality elements whereby the *l*,*u* relationships of the chiral elements are considered in pairs.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2211

l

1. An obsolete prefix for (−)-,
   See: *d*, *l*, *dl*
2. ***See:*** *l*,*u*, for like and unlike diastereoisomers

   Source:
   PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2211

label

A marker, tag or indicator distinguishable by the observer but not by the system and used to identify a tracer.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

labelling

Providing a substance with a label.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

labile

The term has loosely been used to describe a relatively unstable and transient chemical species or (less commonly) a relatively stable but reactive species. It must therefore not be used without explanation of the intended meaning.
See also: inert, persistent, reactive, unreactive

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1134

laboratory sample

The sample or subsample(s) sent to or received by the laboratory. When the laboratory sample is further prepared (reduced) by subdividing, mixing, grinding or by combinations of these operations, the result is the test sample. When no preparation of the laboratory sample is required, the laboratory sample is the test sample. A test portion is removed from the test sample for the performance of the test or for analysis. The laboratory sample is the final sample from the point of view of sample collection but it is the initial sample from the point of view of the laboratory. Several laboratory samples may be prepared and sent to different laboratories or to the same laboratory for different purposes. When sent to the same laboratory, the set is generally considered as a single laboratory sample and is documented as a single sample.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1206
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1465

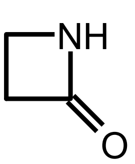
lachrymator

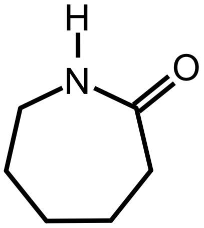
A substance which produces a flow of tears in a person or animal (e.g. acetyl chloride, acrylaldehyde, etc.).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

lactams

Cyclic amides of amino carboxylic acids, having a 1-azacycloalkan-2-one structure, or analogues having unsaturation or heteroatoms replacing one or more carbon atoms of the ring. E.g.

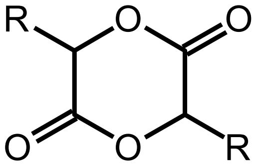




Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1346

lactides

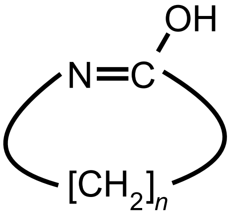
Cyclic esters derived by multiple esterification between two (usually) or more molecules of lactic acid or other hydroxy carboxylic acids They are designated as dilactides, trilactides, etc. according to the number of hydroxy acid residues, e.g. a dilactide (a 1,4-dioxane-2,5-dione):



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1346

lactims

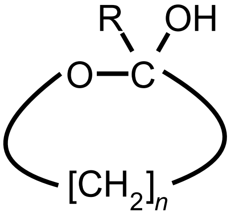
Tautomeric forms of lactams, having an endocyclic carbon-nitrogen double bond. Thus, cyclic carboxamidic acids, e.g.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1346

lactols

1. Cyclic hemiacetals formed by intramolecular addition of a hydroxy group to an aldehydic or ketonic carbonyl group. They are thus 1-oxacy-cycloalkan-2-ols or unsaturated analogues, e.g.

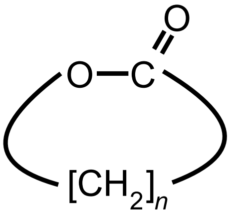


2. [obsolete] This term has also been used for hydroxy lactones, but such use is not recommended.

   Source:
   PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1347

lactones

Cyclic esters of hydroxy carboxylic acids, containing a 1-oxacycloalkan-2-one structure, or analogues having unsaturation or heteroatoms replacing one or more carbon atoms of the ring.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1347

ladder chain

A double-strand chain, consisting of an uninterrupted sequence of rings, with adjacent rings having two or more atoms in common. Alternatively, a ladder chain is a double-strand chain with adjacent constitutional units joined to each other through four atoms, two on one side and two on the other side of each constitutional unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2295

ladder macromolecule

A double-strand macromolecule consisting of an uninterrupted sequence of rings, with adjacent rings having two or more atoms in common. Alternatively, a ladder macromolecule is a double-strand macromolecule with constitutional units joined to each other through four atoms, two on one side and two on the other side of each constitutional unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2295

LADS

Acronym for lifetime-associated difference spectra.
See: global analysis

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 361

lag phase

in biotechnology

The growth interval (adaption phase) between inoculation and start of the exponential phase during which there is little or no growth.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

lambda

Signifies, with its superscript, the bonding number, i.e. the sum of the number of skeletal bonds to an atom and the number of hydrogen atoms associated with it in a parent hydride, real or hypothetical. Its usage in names of compounds is generally restricted to non-standard valence states.

Source:
PAC, 1984, *56*, 769 *(Treatment of variable valence in organic nomenclature (lambda convention) (Recommendations 1983))* on page 774

See also:
Blue Book, p. 465
Red Book, p. 245

Lambert law

The fraction of light absorbed by a system is independent of the incident radiant power (P_λ^0). This law holds only if P_λ^0 is small, scattering is negligible, and multiphoton processes, excited state populations, and photochemical reactions are negligible.
See: absorbance, Beer–Lambert law

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2251

lamellar crystal

A type of crystal with a large extension in two dimensions and a uniform thickness. A lamellar crystal is usually of a thickness in the $5 - 50\ \mathrm{nm}$ range, and it may be found individually or in aggregates. The parallel chain stems intersect the lamellar plane at an angle between $45\ °$ and $90\ °$. The lamellae often have pyramidal shape owing to differences in the fold domains; as a result, one can deduce different fold planes and fold surfaces from the lamellar morphology.

Source:
Purple Book, p. 81

lamp

A source of incoherent radiation.
See: high-pressure mercury lamp (arc), medium-pressure mercury lamp (arc), low-pressure mercury lamp (arc), antimony–xenon lamp (arc), quartz-iodine lamp, resonance lamp, xenon lamp

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2251

lamp black

A special type of carbon black produced by incomplete combustion of a fuel rich in aromatics that is burned in flat pans. Lamp black is characterized by a relatively broad particle size distribution.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 496

Landau–Zener model

Within the Born–Oppenheimer approximation, a semi-classical model for the probability, P, of hopping from one electronic state to another of the same or different *multiplicity*

$$P = \exp\left(- \frac{4\,\pi^2\,{\varepsilon_{12}}^2}{h\,v\ \mid s_1 - s_2 \mid} \right)$$

where ε_{12} is the potential energy gap between the two electronic states at a surface crossing point, $\mid s_1 - s_2 \mid$ is the difference in slopes between the intersecting potential energy curves at this point and v is the nuclear relative velocity with which the system passes the point of closest approach.
Note:

The original formalism only considered states of the same spin multiplicity.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 362

Landolt reaction

A slow chemical reaction, in which the formation of a product is delayed by a suitable reagent added for the purpose.

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2296

Langmuir monolayer [obsolete]

See: monolayer

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1672

Langmuir–Blodgett (LB) membrane

Synthetic composite membrane formed by sequential depositing of one or more monolayers of surface-active component onto a porous or non-porous support.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1482

Langmuir–Hinshelwood mechanism

A mechanism for surface catalysis in which the reaction occurs between species that are adsorbed on the surface is often known as a Langmuir–Hinshelwood mechanism.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 171

Langmuir–Rideal (Rideal–Eley) mechanism

A mechanism for surface catalysis in which the reaction occurs between a reactant molecule in the gas phase and one that is adsorbed on the surface.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 171

Laporte rule

This rule states that for monophotonic radiative transitions in centrosymmetric systems, the only non-vanishing electric-dipole transition moments are those which connect an even term (g) with an odd term (u).

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2251

lapse rate

in atmospheric chemistry

The variation of an atmospheric variable with height; unless otherwise stated the variable is temperature.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

large particle

in radiation scattering

A particle with dimensions comparable with the wavelength of the radiation in the medium or larger. In practice a particle must be treated as large if its largest dimension exceeds about one-twentieth of the wavelength employed.

Source:
Purple Book, p. 65

lariat ethers

Crown ethers (***See:*** crown) having a side chain that holds one or more additional coordinating sites.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1347

See also:
PAC, 1988, *60*, 461 *(Lariat ethers: from cation complexation to supramolecular assemblies)* on page 461

LAS

Acronym for lifetime-associated spectra.
See: global analysis

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 362

laser

A source of ultraviolet, visible, or infrared radiation which produces light amplification by stimulated emission of radiation from which the acronym is derived. The light emitted is coherent except for superradiance emission. The essential elements of a laser are: 1, an active medium; 2, a pumping process to make a population inversion; and 3, suitable geometry of optical feedback elements. The active medium consists of a host material (gas, liquid or solid) containing an active species.
See: argon ion laser, atomic laser, crystal laser, glass laser, ion laser, molecular laser, organic dye laser, helium–cadmium laser, chemical laser, CO_2 laser, copper vapour laser, diode laser, dye laser, excimer laser, free electron laser, free-running laser, gas laser, helium–neon laser, krypton ion laser, mode-locked laser, neodymium laser, nitrogen laser, Q-switched laser, solid-state lasers, ruby laser
.
See also: lasing

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2251
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1915

laser beam ionization

Ionization by irradiation of a specimen with a laser beam.

Source:
Orange Book, p. 204

laser dye

Organic dyes typically used dissolved in an organic solvent. The dye solution is circulated continuously through the laser chamber of the dye laser, in which it is excited (pumped) by flash lamps or by another laser.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 362

laser ionization

in mass spectrometry

Occurs when a sample is irradiated with a laser beam. In the irradiation of gaseous samples, ionization occurs *via* a single- or multi-photon process. In the case of solid samples, ionization occurs *via* a thermal process.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548
Orange Book, p. 204

laser micro emission spectroscopy (LAMES)

Any technique in which a specimen is bombarded with a finely focused laser beam (diameter less than $10\ \mu m$) in the ultraviolet or visible range under conditions of vapourization and thermal excitation of electronic states of sample material and in which the photon emission spectrum is observed.

Source:
Orange Book, p. 250

laser micro mass spectrometry (LAMMS)

Any technique in which a specimen is bombarded with a finely focused laser beam (diameter less than $10\ \mu m$) in the ultraviolet or visible range under conditions of vapourization and ionization of sample material and in which the ions generated are recorded with a mass spectrometer.

Source:
Orange Book, p. 250

laser Raman microanalysis (LRMA)

Any technique in which a specimen is bombarded with a finely focused laser beam (diameter less than $10\ \mu m$) in the ultraviolet or visible range and the intensity versus wavelength function of the Raman radiation is recorded yielding information about vibrational states of the excited substance and therefore also about functional groups and chemical bonding.

Source:
Orange Book, p. 249

laser-jet photochemical technique

Technique by which high concentrations of excited states are generated in a jet, permitting the readily determination of spectroscopic properties of those states.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 363

lasing

The process of light amplification by stimulated emission of radiation.
See: laser

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2251

latent image

The primary result of radiation absorption in a photoimaging system which is susceptible to development.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2251

latent period (latency)

in medicinal chemistry

1. Delay between exposure to a harmful substance and the manifestations of a disease or other adverse effects.
2. Period from disease initiation to disease detection.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1055

lateral order

in a polymer

Order in the side-by-side packing of the molecules of a linear polymer.

Source:
Purple Book, p. 46

lateral resolution

in in situ microanalysis

For qualitative analysis, this should be defined as the minimum distance of two points (areas) on the specimen corresponding to signal levels of 16 and 84%. For electron signals originating from top surface layers like secondary or Auger electrons and secondary ions the lateral resolution for qualitative purposes corresponds to the beam diameter. For signals originating in a greater depth of the sample (back scattered electrons, X-rays) the lateral resolution is worse than the corresponding value of the beam diameter due to the diffusion of the primary electrons. The lateral resolution may be determined exactly with a sandwich specimen or a sharp edge specimen, or approximately with a specimen showing a regular microstructure of known dimensions. Recommended abbreviation: Lat.

Res. (qualitative); unit: m; range: nm or μm. For quantitative analysis, this should be defined as the minimum distance of two points (areas) on the specimen corresponding to signal ratios of 10^4. This condition assures that the value for the lateral resolution defines the diameter of the analytical area which yields the total analytical signal. Due to the effect of electron diffusion in a solid and 'tail effects' in ion beam analysis the quantitative lateral resolution is significantly larger than the beam diameter. Recommended abbreviation: Lat. Res. (quantitative); unit: m; range: nm or μm.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2027

latex

An emulsion or sol in which each colloidal particle contains a number of macromolecules.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 606

lath crystal

A lamellar crystal prevailingly extended along one lateral dimension.

Source:
Purple Book, p. 81

lattice distortion

Structural disorder resulting from misalignment of the unit cells within the crystals.

Source:
Purple Book, p. 80

laws of distribution

Also contains definition of: logarithmic distribution coefficient *in precipitation*

in precipitation

During the formation of a mixed crystal from a solution containing two components 'A' and 'B', the latter may be distributed according to the equation

$$K_{\mathrm{A,B}} = \frac{b\,(a_0 - a)}{a\,(b_0 - b)}.$$

In this homogeneous distribution, a_0 and b_0 are the respective concentrations in the solution before crystallization and a and b are the respective concentrations in the solution after crystallization. $K_{\mathrm{A,B}}$ is usually called the separation factor. The term homogeneous distribution coefficient is not recommended. Alternatively the distribution of the micro-component may follow the equation of Doerner and Hoskins

$$\ln\left(\frac{a_0}{a}\right) = \lambda \ln\left(\frac{b_0}{b}\right)$$

(logarithmic distribution) where λ is usually called the logarithmic distribution coefficient, the meaning of the other symbols remaining the same. Exactly homogeneous or logarithmic distributions are extreme cases and very seldom encountered.

Source:
Orange Book, p. 85

layer

Also contains definition of: double-layer

Any conceptual region of space restricted in one dimension, within or at the surface of a condensed phase or a film. The usage of the term 'film' for an adsorption layer is confusing and is discouraged. The term double-layer applies to layers approximated by two 'distinct' sublayers.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1671

layer equilibrium

in chromatography

Saturation of the stationary phase with the mobile phase via the vapour phase.

Source:
Orange Book, p. 99

leader sequence

Also contains definition of: signal sequence

in biotechnology

1. A polynucleotide region between promoter and structural gene, necessary for the correct transcription of DNA into mRNA.
2. An N-terminal extension of polypeptides (also known as the signal sequence) which is necessary for the transport of the protein into or through the membrane or for its secretion into the extracellular medium.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

least motion, principle of

The statement that those elementary reactions are the most favoured which exhibit the fewest possible alterations in the positions of the atomic nuclei and in the electronic configuration. The most frequently used mathematical formulation of the principle rests on a mechanical model of a molecule in which the energy of structural deformation, when reactants (r) turn into products (p), is assumed to be proportional to the sum of the squares of the changes in the positions of the nuclei common to both reactants and products

$$E = \sum_i f_i \,(q^{\mathrm{p}_i} - q^{\mathrm{r}_i})^2$$

where f_i is the force constant (in many applications set equal to unity). The equation coincides with the relationship for the potential energy of small vibrations, hence it is valid only at a very early stage of a reaction. This is one of the reasons why many reactions violate the principle of least motion.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1949

least-squares technique

A procedure for replacing the discrete set of results obtained from an experiment by a continuous function. It is defined by the following. For the set of variables y, x_0, x_1, ... there are n measured values such as y_i, x_{0i}, x_{1i}, ... and it is decided to write a relation:

$$y = f(a_0, a_1, ..., a_K; x_0, x_1, ...)$$

where a_0, a_1, ..., a_K are undetermined constants. If it is assumed that each measurement y_i of y has associated with it a number w_i^{-1} characteristic of the uncertainty, then numerical estimates of the a_0, a_1, ..., a_K are found by constructing a variable S, defined by

$$S = \sum_i (w_i \,(y_i - f_i))^2,$$

and solving the equations obtained by writing

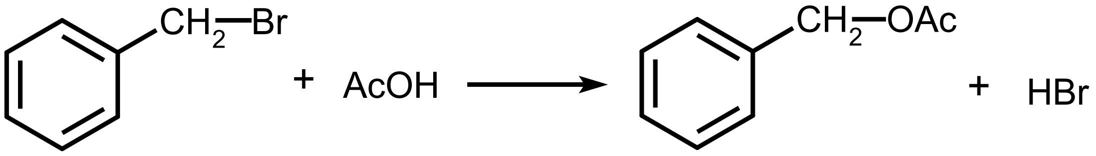
$$\frac{\partial S}{\partial a_j} \tilde{a}_j = 0$$

$\tilde{a}_j =$ all a except a_j. If the relations between the a and y are linear, this is the familiar least-squares technique of fitting an equation to a number of experimental points. If the relations between the a and y are non-linear, there is an increase in the difficulty of finding a solution, but the problem is essentially unchanged.

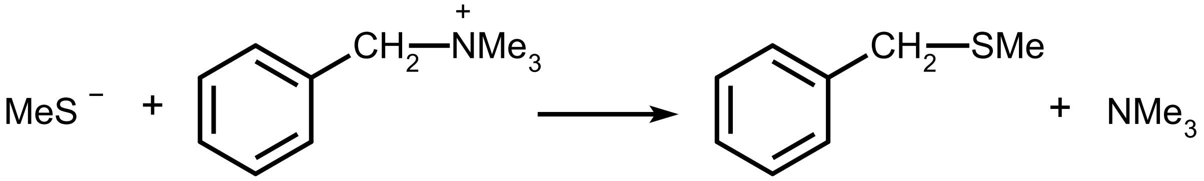
Source:
PAC, 1981, *53*, 1805 *(Assignment and presentation of uncertainties of the numerical results of thermodynamic measurements (Provisional))* on page 1822

leaving group

An atom or group (charged or uncharged) that becomes detached from an atom in what is considered to be the residual or main part of the substrate in a specified reaction. For example, in the heterolytic solvolysis of benzyl bromide in acetic acid:



the leaving group is Br^-; in the reaction:

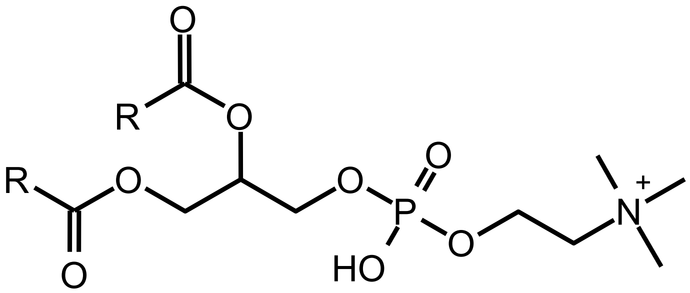


the leaving group is NMe_3 ; in the electrophilic nitration of benzene, it is H^+. The term has meaning only in relation to a specified reaction. The leaving group is not, in general, the same as the substituent group present in the substrate (e.g. bromo and trimethylammonio in the substrates of the first two examples above.) A slightly different usage of the term prevails in the (non-mechanistic) naming of transformations, where the actual substituent group present in the substrate (and also in the product) is referred to as the leaving group.
See also: electrofuge, entering group, nucleofuge

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1134

lecithins

Choline esters of phosphatidic acids. Specific compounds should be named systematically.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1347

See also:
White Book, p. 184

lectins

Glycoproteins isolated from plants but recently found also in animals and microorganisms that react specifically with terminal glycosidic residues of other molecules (e.g. cell wall polysaccharides); some causing cells to agglutinate (cf. agglutination).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

LED

Acronym for light-emitting diode.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 363

left-to-right convention

Arrangement of the structural formulae of the reactants so that the bonds to be made or broken form a linear array in which the electrons move from left to right.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1134

length, l

Base quantity in the system of quantities upon which SI is based. Special symbols are used for different types of lengths.

Source:
Green Book, 2nd ed., p. 11
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 978

lethal concentration

Concentration of a potentially toxic substance in an environmental medium that causes death following a certain period of exposure (denoted by LC).
See also: lethal dose

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2063

lethal dose

Amount of a substance or physical agent (radiation) that causes death when taken into the body by a single absorption (denoted by LD).
See also: lethal concentration

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2063

lethal synthesis

Synonym: suicide metabolism

Metabolic formation of a highly toxic compound from one that is relatively non-toxic (bioactivation), often leading to death of affected cells. Synonymous with suicide metabolism.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2063

leuco bases

Colourless compounds formed by reduction of triphenylmethane dyes. Generally, they are amino or hydroxy derivatives of triphenylmethane. Use of this class name, which is more or less parochial to the technology of dyes, is not endorsed. E.g. $(p\text{-}Me_2NC_6H_4)_2CHPh$, the leuco base of Malachite Green.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1347

leuco compounds [obsolete]

Dihydroxy polycyclic aromatic compounds which on oxidation form polycyclic quinone dyes (intermediates in vat dyeing). Use of this class name, which is more or less parochial to the technology of dyes, is not endorsed.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1347

leukotrienes

Linear C_{20} endogenous metabolites of arachidonic acid (icosa-5,8,11,14-tetraenoic acid) containing a terminal carboxy function and four or more double bonds (three or more of which are conjugated) as well as other functional groups. A subclass of icosanoids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1347

level

Logarithm of the ratio of a quantity and a reference value of that quantity.
See: field level, power level

Source:
Green Book, 2nd ed., p. 79

level width, Γ

Planck constant over $2\,\pi$ divided by the mean life.

Source:
Green Book, 2nd ed., p. 22

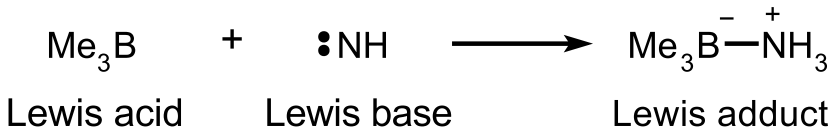
levelling effect

The tendency of a solvent to make all Brønsted acids whose acidity exceeds a certain value appear equally acidic. It is due to the complete transfer to a protophilic solvent of a hydron from a dissolved acid stronger than the conjugate acid of the solvent. The only acid present to any significant extent in all such solutions is the lyonium ion. For example, the solvent water has a levelling effect on the acidities of $HClO_4$, HCl and HI : aqueous solutions of these acids at the same (moderately low) concentrations have the same acidities. A corresponding levelling effect applies to strong bases protogenic solvents.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1135

Lewis acid

A molecular entity (and the corresponding chemical species) that is an electron-pair acceptor and therefore able to react with a Lewis base to form a Lewis adduct, by sharing the electron pair furnished by the Lewis base. For example:



See also: coordination, dipolar bond

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1135

Lewis acidity

The thermodynamic tendency of a substrate to act as a Lewis acid. Comparative measures of this property are provided by the equilibrium constants for Lewis adduct formation of a series of Lewis acids with a common reference Lewis base.
See also: acceptor number (AN), electrophilicity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1135

Lewis adduct

The adduct formed between a Lewis acid and a Lewis base.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1135

Lewis base

A molecular entity (and the corresponding chemical species) able to provide a pair of electrons and thus capable of coordination to a Lewis acid, thereby producing a Lewis adduct.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1135

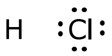
Lewis basicity

The thermodynamic tendency of a substance to act as a Lewis base. Comparative measures of this property are provided by the equilibrium constants for Lewis adduct formation for a series of Lewis bases with a common reference Lewis acid.
See also: donor number (DN), nucleophilicity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1135

Lewis formula (electron dot or Lewis structure)

Molecular structure in which the valency electrons are shown as dots so placed between the bonded atoms that one pair of dots represents two electrons or one covalent (single) bond, e.g.



A double bond is represented by two pairs of dots, etc. Dots representing non-bonded outer-shell electrons are placed adjacent to the atoms with which they are associated, but not between the atoms. Formal charges (e.g. +, −, 2+, etc.) are attached to atoms to indicate the difference between the positive nuclear charge (atomic number) and the total number of electrons (including those in the inner shells), on the formal basis that bonding electrons are shared equally between atoms they join. (Bonding pairs of electrons are usually denoted by lines, representing covalent bonds, as in line formulae.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1135

Lewis octet rule

A classical rule for describing the electronic configuration of atoms in molecules: the maximum number of electron pairs that can be accommodated in the valence shell of a first-row element is four. For the second and subsequent row elements there are many exceptions to this rule.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1949

LIDAR

in atmospheric chemistry

An acronym for Light Detection And Ranging. It is a real time remote sensing technique for the determination of aerosol and trace gas concentrations in air by measurement of scattered laser radiation.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

lifetime

of luminescence

The time required for the luminescence intensity to decay from some initial value to $\frac{1}{\mathrm{e}}$ of that value ($\mathrm{e} = 2.718 \ldots$). Lifetimes can be measured by phase fluorimetry (phosphorimetry) where the phase shift between the sinusoidally modulated exciting light and the emitted light is measured.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 242

lifetime, τ

Also contains definition of: mean lifetime, τ

Lifetime of a molecular entity, which decays by first-order kinetics, is the time needed for a concentration of the entity to decrease to $1/\mathrm{e}$ of its original value, *i.e.*, $c(t = \tau) = \frac{c(t = 0)}{\mathrm{e}}$. Statistically, it represents the life expectation of the entity. It is equal to the reciprocal of the sum of the first-order rate constants of all processes causing the decay of the molecular entity.
Notes:

1. Mathematical definition: $\tau = \frac{1}{k} = \frac{1}{\sum_i k_i}$ with k_i the first-order rate constants for all decay processes of the decaying state.
2. Lifetime is used sometimes for processes, which are not first order. However, in such cases, the lifetime depends on the initial concentration of the entity, or of a quencher and, therefore, only an initial or a mean lifetime can be defined. In this case it should be called *decay time*.
3. Occasionally, the term *half-life* ($\tau_{1/2}$) is used, representing the time needed for the concentration of an entity to decrease to one half of its original value, *i.e.*, $c(t = \tau_{1/2}) = \frac{c(t = 0)}{2}$. For first-order reactions, $\tau_{1/2} = \ln 2\, \tau$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 363

ligand field

Ligand field theory is a modified crystal field theory that assigns certain parameters as variables rather than taking them as equal to the values found for free ions, thereby taking into account the potential covalent character of the metal-ligand bond.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1283

ligand field splitting

The removal of a degeneracy of atomic or molecular levels in a molecule or ion with a given symmetry, induced by the attachment or removal of ligands to produce reduced symmetries.
See: crystal field splitting

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2251

ligand to ligand charge transfer (LLCT) transition

An electronic transition of a metal complex that corresponds to excitation populating an electronic state in which considerable electron transfer between two ligands has occurred.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2252

ligand to metal charge transfer (LMCT) transition

An electronic transition in a metal complex that corresponds to excitation populating an electronic state in which considerable electron transfer from a ligand to a metal centre has occurred.
See also: metal to ligand charge transfer transition

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2252

ligands

1. In an inorganic coordination entity, the atoms or groups joined to the central atom.

   Source:
   Red Book, p. 146
2. In biochemistry: if it is possible or convenient to regard <u>part</u> of a polyatomic molecular entity as central, then the atoms, groups or molecules bound to that part are called ligands. Biochemical usage is thus wider, in that the central entity can be polyatomic. Thus H^+ may be a ligand for proteins and for citrate as well as for O^{2-} . It may even be a ligand for a univalent entity such as acetate: in other circumstances, AcO^- may be the ligand for H^+, since the definition makes it clear that the view of which entity is central may change for convenience. Thus, four calcium ions are ligands for calmodulin, when the protein is regarded as central: four carboxylate groups of calmodulin ligate (are ligands of) each calcium ion when this ion is regarded as central. It is the ligand that is said to ligate the central entity, which is said to be ligated. When the hormone binding to a receptor is called a ligand, the receptor is thus regarded as the central entity. Biochemists should bear in mind that the usage in inorganic chemistry has been that ligands bind only single atoms, so they should be cautious in fields such as bioinorganic chemistry where confusion may be possible.

Source:
White Book, p. 335
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1136

ligases (synthetases)

Enzymes that catalyse the ligation of two molecules with concomitant hydrolysis of the pyrophosphate bond in adenosine 5'-triphosphate (ATP) or a similar triphosphate, forming C–C , C–O , C–S , P–O or C–N bonds. In recombinant DNA technology, ligases covalently join together two sequences of DNA (e.g. host DNA and foreign DNA) by a phosphodiester bond.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 159

ligate

To coordinate to a central atom as a ligand.

Source:
Red Book, p. 146

light polarization

A light beam is said to be linearly polarized if the end-point of the electric vector moves in a straight line when viewed along the direction of propagation of the beam. If it moves along a circle the beam is circularly polarized and if it moves along an ellipse the beam is elliptically polarized.
Note:
Circular polarization is said to be right-handed if the direction of rotation is clockwise when viewed against the direction of propagation and left-handed if the sense of the rotation is opposite. When the position of the endpoint of the electric vector is viewed at a given time t as a function of distance along x, it forms a left-handed helix if the light polarization is left-handed and a right-handed helix is it is right-handed.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 364

light scattering

The redirection of a light beam due to interactions with molecules (Rayleigh and Raman scattering) and aerosols (Mie scattering). Scattered light received at any point in the atmosphere (sometimes called *sky* radiation) is a very important component of the total radiation received from the sun; it is dependent on the solar zenith angle, elevation aerosol concentration etc.
See also: elastic scattering

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

light source

See: lamp, laser

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2252

light-atom anomaly

A dynamical effect that arises for a process

$$\mathrm{A} + \mathrm{B{-}C} \longrightarrow \mathrm{A{-}B} + \mathrm{C}$$

when the species A is light (e.g. a hydrogen atom) compared to B and C . The vibrational excitation of the product A–B is low, since the light atom A approaches to within the bonding distance of BC before the C atom retreats. The energy of reaction is therefore released as repulsion between A–B and C , with the result that there is translational excitation of the products.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 171

light-emitting diode (LED)

Semiconductor (often a combination of gallium, arsenic and phosphorous or gallium and nitrogen) containing an *n* region (where electrons are more numerous than positive charges) separated from a *p* region (where positive charges are more numerous than negative charges). Upon application of a voltage, charges move and emission of ultraviolet, visible or infrared radiation is produced each time a charge recombination takes place. Although a LED emits incoherent monochromatic light, normally a very narrow frequency range is obtained.
Notes:

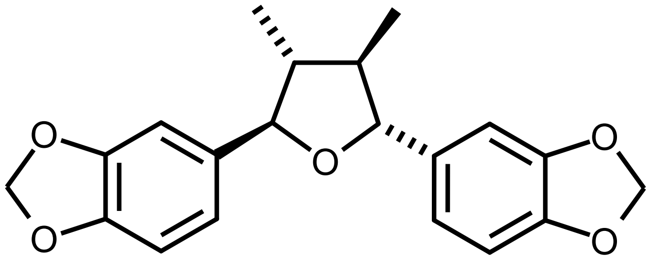
1. This effect is a form of electroluminescence.
2. The colour depends on the semi-conducting material used, and can be ultraviolet, visible or infrared.
3. Organic light-emitting devices (OLEDs) contain diodes made of small molecules or made of polymeric materials. The latter are sometimes called PLEDs.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 364

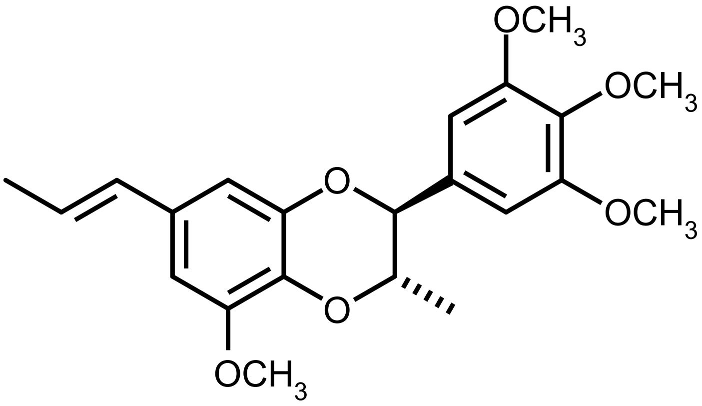
lignans

Also contains definition of: neolignans

Plant products of low molecular weight formed primarily from oxidative coupling of two *p*-propylphenol moieties at their β carbon atoms; products with units coupled in other ways are neolignans, e.g.



galbacin, a lignan



(−)-eusiderin, a neolignan

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1347

lignins

Macromolecular constituents of wood related to lignans, composed of phenolic propylbenzene skeletal units, linked at various sites and apparently randomly.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

limit of detection

in analysis

The limit of detection, expressed as the concentration, c_{L}, or the quantity, q_{L}, is derived from the smallest measure, x_{L}, that can be detected with reasonable certainty for a given analytical procedure. The value of x_{L} is given by the equation

$$x_{\mathrm{L}} = \bar{x}_{\mathrm{bi}} + k\, s_{\mathrm{bi}}$$

where $\bar{x}_{\mathrm{bi}}$ is the mean of the blank measures, s_{bi} is the standard deviation of the blank measures, and k is a numerical factor chosen according to the confidence level desired.

Source:
Orange Book, p. 5

limit test

in toxicology

Acute toxicity test in which, if no ill-effects occur at a pre-selected maximum dose, no further testing at greater exposure levels is required.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2063

limiting adsorption current

The potential-independent value that is approached by an adsorption current as the rate of reduction or oxidation of the electroactive substance is increased by varying the applied potential. The terms adsorption current and limiting adsorption current should not be applied to faradaic currents that have been increased or decreased by adding a non-electroactive surfactant to a solution containing an electroactive substance, nor to apparent waves resulting from the effect of adsorption or desorption on double-layer currents.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1494

limiting catalytic current

The potential-independent value that is approached by a catalytic current as the rate of the charge-transfer process is increased by varying the applied potential.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1495

limiting condition of operation

Range of physical and operational parameters in which the method meets given values of performance characteristics with 95% probability.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

limiting current

The limiting value of a faradaic current that is approached as the rate of the charge-transfer process is increased by varying the potential. It is independent of the applied potential over a finite range, and is usually evaluated by subtracting the appropriate residual current from the measured total current. A limiting current may have the character of an adsorption, catalytic, diffusion, or kinetic current, and may include a migration current.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 513
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1497

limiting diffusion current

The potential-independent value that is approached by a diffusion current as the rate of the charge-transfer process is increased by varying the applied potential.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1495

limiting kinetic current

The potential-independent value that is approached by a kinetic current as the rate of the charge-transfer process is increased by varying the applied potential.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1497

limiting migration current

The limiting value of a migration current, which is approached as the rate of the charge-transfer process is increased by varying the applied potential.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1498

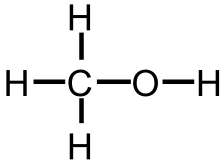
limiting sedimentation coefficient

See: sedimentation coefficient

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 616

line formula

A two-dimensional representation of molecular entities in which atoms are shown joined by lines representing single or multiple bonds, without any indication or implication concerning the spatial direction of bonds. For example, methanol is represented as:



$$\mathrm{H{-}\overset{H}{\underset{H}{C}}{-}O{-}H}$$

(The term should not be confused with the representation of chemical formulae by the 'Wiswesser line notation', a method of string notation. Formulae in this notation are also known as 'Wiswesser line formulae'.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1136

line repetition groups

The possible symmetries of arrays extending in one direction with a fixed repeating distance. Linear polymer chains in the crystalline state must belong to one of the line repetition groups. Permitted symmetry elements are: the identity operation (symbol 1); the translation along the chain axis (symbol t); the mirror plane orthogonal to the chain axis (symbol m) and that containing the chain axis (symbol d); the glide plane containing the chain axis (symbol c); the inversion centre, placed on the chain axis (symbol i); the two-fold axis orthogonal to the chain axis (symbol 2); the helical, or screw, symmetry where the axis of the helix coincides with the chain axis. In the latter case, the symbol is $\mathrm{s}\,(A * M / N)$, where s stands for the screw axis, A is the class of the helix, * and / are separators, and M is the integral number of residues contained in N turns, corresponding to the identity period (M and N must be prime to each other). The class index A may be dropped if deemed unnecessary, so that the helix may also be simply denoted as $\mathrm{s}\,(M / N)$.

Source:
Purple Book, p. 79

line width

Width of a spectral line in terms of wavelength, frequency or wavenumber. Usually defined as full or half width of the line at half of the maximum intensity FWHM or HWHM, respectively).

Source:
Green Book, 2nd ed., p. 31

line width

in Mössbauer spectroscopy

The full width at half maximum peak-height. The natural linewidth is the theoretical value of the full width at half maximum of the nuclear transition, usually calculated from lifetime data.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 213

line-of-centres model

A form of the collision theory of chemical reactions in which the assumption is made that reaction can only occur if on collision the component of energy along the line of centres of the masses of the colliding species is greater than a particular threshold energy.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 171

line-shape analysis

Determination of rate constants for a chemical exchange from the shapes of spectroscopic lines of dynamic processes. The method is most often used in nuclear magnetic resonance spectroscopy.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1136

linear absorption coefficient

See: absorption coefficient

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 978

linear attenuation coefficient

See: attenuation coefficient

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 978

linear chain

A chain with no branch points intermediate between the boundary units.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2293

linear chromatography

Chromatographic process, where the retention is governed by a linear distribution isotherm.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1593

linear copolymer

A copolymer composed of linear macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2303

linear (decadic) absorption coefficient

in optical spectroscopy

See: absorption coefficient

Source:
Green Book, 2nd ed., p. 32

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2169
PAC, 1988, *60*, 1055 *(Glossary of terms used in photochemistry (Recommendations 1988))* on page 1058
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 959

linear (decadic) attenuation coefficient

in optical spectroscopy

See: attenuation coefficient

Source:
Green Book, 2nd ed., p. 32

See also:
Orange Book, p. 212
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 963

linear dichroism (LD)

For a uniaxial sample with sample axis Z is defined as:

$$\Delta A_\mathrm{l} = A_Z - A_Y$$

where A_Z and A_Y are the absorption spectra measured with the electric vector of linearly polarized light along and perpendicular to the sample axis, respectively. For an isotropic sample $\Delta A_\mathrm{l} = 0$.

Notes:

1. Sometimes the reduced dichroism is used instead. It is defined as

   $$\Delta A_\mathrm{r} = \frac{A_Z - A_Y}{A_Z + 2\,A_Y} = \frac{A_Z - A_Y}{3\,A_\mathrm{iso}}$$

   with A_iso the isotropic absorbance. Thus, ΔA_r is analogous to emission anisotropy and the denominator in the equation corresponds to three times the absorbance measured in a similar but isotropic sample.
2. The dichroic ratio $d(\lambda)$ is also a frequently used function of the wavelength. It is defined as

   $$d(\lambda) = \frac{A_Z}{A_Y}$$
3. Most naturally-occurring solid samples exhibit linear dichroism. It may also be produced in the laboratory by dissolving the sample molecules in anisotropic solvents such as nematic liquid crystals or stretched polymers. This procedure tends to produce uniaxial samples. Also crystals may be used as aligned solvents and if the sample forms suitable crystals by itself these may be used directly. Other molecular alignment techniques include application of electric or magnetic fields.
4. Photoselection is a commonly used technique for the production of aligned samples; both the photoselected subset and the set of remaining molecules may be studied.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 365

linear dispersion

See: dispersion (for spectroscopic instruments)

Source:
Orange Book, p. 158

linear distribution isotherm

in chromatography

A distribution isotherm which can be approximated as $c_S = K_C \cdot c_M$ where K_C is a constant.

Note:
At low concentrations, all distribution isotherms tend towards being linear. K_C is the distribution constant.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1593

linear electron accelerator

An evacuated metal tube in which electrons pass through a series of small gaps (usually) in the form of cavity resonators in the high frequency range) so arranged and spaced that, at a specific excitation frequency, the stream of electrons on passing through successive gaps gains additional energy from the electric field in each gap.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1545

linear energy transfer

The average energy locally imparted to a medium by a charged particle of specified energy, per unit distance traversed.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1545

linear free-energy relation

Also contains definition of: linear Gibbs energy relation

A linear correlation between the logarithm of a rate constant or equilibrium constant for one series of reactions and the logarithm of the rate constant or equilibrium constant for a related series of reactions. Typical examples of such relations (also known as linear Gibbs energy relations) are the Brønsted relation, and the Hammett equation (***See also:*** σ-constant).
The name arises because the logarithm of an equilibrium constant (at constant temperature and pressure) is proportional to a standard free energy (Gibbs energy) change, and the logarithm of a rate constant is a linear function of the free energy (Gibbs energy) of activation.

It has been suggested that this name should be replaced by linear Gibbs energy relation, but at present there is little sign of acceptance of this change.
The area of physical organic chemistry which deals with such relations is commonly referred to as 'Linear Free-Energy Relationships'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1136

linear macromolecule

A macromolecule the structure of which essentially comprises the multiple repetition in linear sequence of units derived, actually or conceptually, from molecules of low relative molecular mass.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2290

linear polarizer

An optical device which allows the transmission of radiation of which the electric vector is restricted to one plane resulting in linearly polarized radiation.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 238

linear polymer

A polymer composed of linear macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2303

linear pulse amplifier

A pulse amplifier which, within the limits of its normal operating characteristics, delivers an output pulse of amplitude proportional to that of the input pulse.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

linear range

Concentration range over which the intensity of the signal obtained is directly proportional to the concentration of the species producing the signal.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

linear solvation energy relationships

Equations involving the application of solvent parameters in linear or multiple (linear) regression expressing the solvent effect on the rate or equilibrium constant of a reaction.
See: Dimroth–Reichardt E_T parameter, Kamlet–Taft solvent parameter, Koppel–Palm solvent parameter, Z-value

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1136

linear strain, ε, e

Change of length divided by the original length.

Source:
Green Book, 2nd ed., p. 12

linearity of responsivity (of a radiation detector)

The extent to which the output of the detector is directly proportional to the incident radiant power at a given wavelength and at constant irradiation geometry.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1750

lineic

Attribute to a physical quantity obtained by division by length. Lineic mass of a thread is the mass of the thread divided by its length.

Source:
ISO 31-0: 1992 *(Quantities and Units - Part 0: General Principles, Units and Symbols.)*
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 978

Lineweaver–Burk plot

A plot of the reciprocal of velocity of an enzyme-catalysed reaction (ordinate) versus the reciprocal of substrate concentration (abscissa). The plot is used to graphically define the maximum velocity of an enzyme-catalysed reaction and the Michaelis constant for the enzyme.
See also: Michaelis–Menten kinetics

Source:
PAC, 1994, *66*, 2587 *(Glossary of bioanalytical nomenclature - Part 1: General terminology, body fluids, enzymology, immunology (IUPAC Recommendations 1994))* on page 2593

linked scan

in mass spectrometry

A scan, in an instrument comprising two or more analysers, in which two or more of the analyser fields are scanned simultaneously so as to preserve a pre-determined relationship between parameters characterizing these fields. Often, these parameters are the field strengths, but they may also be the frequencies in the case of analysers in which alternating fields are employed.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1551

lipid film

Established term for W/O/W films (i.e. oil film in water).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

lipids

A loosely defined term for substances of biological origin that are soluble in nonpolar solvents. They consist of saponifiable lipids, such as glycerides (fats and oils) and phospholipids, as well as nonsaponifiable lipids, principally steroids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

See also:
White Book, p. 180

lipophilic

Literally 'fat-loving'. Applied to molecular entities (or parts of molecular entities) having a tendency to dissolve in fat-like (e.g. hydrocarbon) solvents.
See also: hydrophilic, hydrophobic interaction, lyophilic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1136
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

lipophilicity

Lipophilicity represents the affinity of a molecule or a moiety for a lipophilic environment. It is commonly measured by its distribution behaviour in a biphasic system, either liquid-liquid (*e.g.*, partition coefficient in 1-octanol/water) or solid-liquid (retention on reversed-phase high-performance liquid chromatography (*RP-HPLC*) or thin-layer chromatography (*TLC*) system).

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1145
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1123
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

lipophobic

Literally, 'fat-rejecting'; the converse of lipophilic.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

lipopolysaccharides

Natural compounds consisting of a trisaccharide repeating unit (two heptose units and octulosonic acid) with oligosaccharide side chains and 3-hydroxytetradecanoic acid units (they are a major constituent of the cell walls of Gram-negative bacteria).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

lipoproteins

Clathrate complexes consisting of a lipid enwrapped in a protein host without covalent binding in such a way that the complex has a hydrophilic outer surface consisting of all the protein and the polar ends of any phospholipids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

liposome

Originally a lipid droplet in the endoplasmic reticulum of a fatty liver. Now applied to an artificially formed lipid droplet, small enough to form a relatively stable suspension in aqueous media and with potential use in drug delivery.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2064

Lippman's equation

An equation which gives the electric charge per unit area of an interface (electrode):

$$\left(\frac{\partial \gamma}{\partial E_{\mathrm{A}}}\right)_{T,p,\mu_i \neq \mu} = -Q_{\mathrm{A}}$$

where γ is the interfacial tension, E_{A} is the potential of a cell in which the reference electrode has an interfacial equilibrium with one of the ionic components of A, Q_{A} is the charge on unit area of the interface, μ_i is the chemical potential of the combination of species i whose net charge is zero, T is the thermodynamic temperature and p is the external pressure. Since more than one type of reference electrode may be chosen, more than one quantity Q may be obtained. Consequently Q cannot be considered as equivalent to the physical charge on a particular region of the interphase. It is in fact an alternative way of expressing a surface excess or combination of surface excess of charged species.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 508
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 445

liquid chromatography (LC)

A separation technique in which the mobile phase is a liquid. Liquid chromatography can be carried out either in a column or on a plane. Present-day liquid chromatography generally utilizing very small particles and a relatively high inlet pressure is often characterized by the term high-performance (or high-pressure) liquid chromatography, and the acronym HPLC.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 825

liquid crystal

A substance in the liquid-crystalline state.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 495

liquid excimer laser

A liquid laser in which excimer species in liquids are used as the active medium.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1921

liquid ion exchange

A term used to describe a liquid-liquid extraction process that involves a transfer of ionic species from the extractant to the aqueous phase in exchange for ions from the aqueous phase. The term does not imply anything concerning the nature of the bonding in the extracted complex. The term solvent ion exchange is not recommended.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2378

liquid ion laser

A liquid laser in which rare earth ions in solution are used as the laser active medium. An example is KrF in liquid Kr laser.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1921

liquid junction

Any junction between two electrolyte solutions of different composition. Across such a junction there arises a potential difference, called the liquid junction potential. In the operational pH cell the junction is between the test, or pH standard, solution and the filling solution or the bridge solution of the reference electrode.

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 541

liquid laser

A laser in which a liquid solution is the active species.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1921

liquid membrane

Liquid phase existing either in supported or unsupported form that serves as a membrane barrier between two phases.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1486

liquid scintillation detector

A scintillation detector in which the test portion is mixed with a liquid scintillator.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

liquid volume

in gas chromatography

That volume occupied by the liquid phase in the column. Defined by

$$V_{\mathrm{L}} = \frac{w_{\mathrm{L}}}{\rho_{\mathrm{L}}}$$

where w_{L} is the weight of the liquid in the column, and ρ_{L} is the density at the column temperature.

Source:
Orange Book, p. 99

liquid-coated stationary phase (material)

in liquid chromatography

A material in which a liquid stationary phase is coated on the surface of the solid support.

Source:
PAC, 1997, *69*, 1475 *(Classification and characterization of stationary phases for liquid chromatography: Part I. Descriptive terminology (IUPAC Recommendations 1997))* on page 1479

liquid-crystal dendrimer

A highly-branched oligomer or polymer of dendritic structure containing mesogenic groups that can display mesophase behaviour.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 506

liquid-crystal polymer

A polymer material that, under suitable conditions of temperature, pressure, and concentration, exists as an LC mesophase.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 502

liquid-crystal state

A mesomorphic state having long-range orientational order and either partial positional order or complete positional disorder.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 495

liquid-crystal transitions

Also contains definitions of: cholesteric phase, nematic phase

A liquid crystal is a molecular crystal with properties that are both solid- and liquid-like. Liquid crystals are composed predominantly of rod-like or disc-like molecules, that can exhibit one or more different, ordered fluid phases as well as the isotropic fluid; the translational order is wholly or partially destroyed but a considerable degree of orientational order is retained on passing from the crystalline to the liquid phase in a mesomorphic transition.

1. Transition to a nematic phase.
   A mesomorphic transition that occurs when a molecular crystal is heated to form a nematic phase in which the mean direction of the molecules is parallel or antiparallel to an axis known as the director.
2. Transition to a cholesteric phase.
   A mesomorphic transition that occurs when a molecular crystal is heated to form a cholesteric phase in which there is simply a spiralling of the local orientational order perpendicular to the long axes of the molecules.
3. Transition to a smectic state.
   A mesomorphic transition that occurs when a molecular crystal is heated to yield a smectic state in which there is a one-dimensional density wave which produces very soft/disordered layers.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 584

liquid-crystalline phase

A phase occurring over a definite temperature range within the liquid-crystalline state.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 495

liquid-crystalline polymer

Also contains definition of: liquid crystal polymer

Polymeric material that, under suitable conditions of temperature, pressure, and concentration, exists as a liquid-crystalline mesophase.
Notes:

1. ***See also:*** liquid crystal.
2. A liquid-crystalline polymer can exhibit one or more liquid state(s) with one- or two-dimensional, long-range orientational order over certain ranges of temperatures either in the melt (thermotropic liquid-crystalline polymer) or in solution (lyotropic liquid-crystalline polymer).

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 900

liquid-gel chromatography

Includes gel-permeation and ion-exchange chromatography. Liquid is the mobile phase, gel the stationary phase.

Source:
Orange Book, p. 93

liquid-liquid distribution (extraction) (partition)

The process of transferring a dissolved substance from one liquid phase to another (immiscible or partially miscible) liquid phase in contact with it. Although extraction, partition and distribution are not synonymous, extraction may replace distribution where appropriate.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2378
Orange Book, p. 87

liquid-liquid extraction

This term may be used in place of liquid-liquid distribution when the emphasis is on the analyte(s) being distributed (or extracted).
Note:
The distinction between the distribution constant (K_{D}) and the partition constant ($K^{\mathrm{o}}_{\mathrm{D}}$) or the concentration distribution ratio (D_{c}) is reaffirmed and it is recommended that the terms partition constant, partition coefficient and extinction constant should not be used as synonyms for the

(analytical) distribution ratio, D_c. A distinction is drawn between the terms solvent and diluent, and the term extractant is now restricted to the active substance in the solvent (i.e. the homogeneous 'organic phase' which comprises the extractant, the diluent and/or the modifier) which is primarily responsible for the transfer of solute from the 'aqueous' to the 'organic' phase.

Source:
Orange Book, p. 88

liquid-phase loading

in chromatography

A term used in partition chromatography to express the relative amount of the liquid stationary phase in the column packing. It is equal to the mass fraction (%) of liquid stationary phase in the total packing (liquid stationary phase plus support).

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831

liquidus

A line on a binary phase diagram (or surface on a ternary phase diagram) that indicates the temperature at which solidification begins on cooling or at which melting is completed on heating under equilibrium conditions.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 585

lithometeor

in atmospheric chemistry

A particle of dry substance in the atmosphere, as contrasted to a hydrometeor.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

lithosphere

in atmospheric chemistry

The crust of the earth, usually thought of as discrete from and in contact with the hydrosphere and the atmosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

litre

Non-SI unit of volume, $\mathrm{L} = 10^{-3}\ \mathrm{m}^3$. The other allowed symbol is l.

Source:
Green Book, 2nd ed., p. 111

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 979
PAC, 1986, *58*, 1405 *(Recommendations for the presentation of thermodynamic and related data in biology (Recommendations 1985))* on page 1407

live time

For a measurement, the time during which a radiation measuring assembly is capable of processing events occurring in the radiation detector. It equals the clock time minus the integrated resolving or dead time (to be distinguished from 'life time').

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

living copolymerization

A copolymerization which is a living polymerization.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2309

living polymer

Polymer with stable, polymerization-active sites formed by a chain polymerization in which irreversible chain transfer and chain termination are absent.
See also: living polymerization.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 896

living polymerization

A chain polymerization from which chain transfer and chain termination are absent. In many cases, the rate of chain initiation is fast compared with the rate of chain propagation, so that the number of kinetic-chain carriers is essentially constant throughout the polymerization.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2308

load (on a precision balance)

The total weight acting, after counterbalancing, upon the terminal bearing which carries the object being weighed.

Source:
Orange Book, p. 35

loading capacity

Synonyms: maximum loading, saturation capacity, saturation loading

in solvent extraction

The maximum concentration of solute(s) that a solvent can contain under specified conditions.
Notes:

1. The terms maximum loading, saturation capacity and saturation loading are synonymous.
2. All the above terms should clearly be distinguished from ultimate capacity.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2384

local conformation

of a polymer

The conformation of a macromolecule at the scale of the constitutional units. In the polymer literature, local conformation is sometimes referred to as microconformation.

Source:
Purple Book, p. 77

local efficiency of atomization, ε_{a}

in flame spectrometry

The substance fraction of atomized component in the component consumed. The efficiency of atomization is measured in a given part of the flame, usually the observation space; $\varepsilon_{\mathrm{a}} = \varepsilon_{\mathrm{n}}\, \chi_{\mathrm{s}}\, \chi_{\mathrm{v}}\, \chi_{\mathrm{a}}$. The signal is a function of the product $q_{\mathrm{v}}\, \varepsilon_{\mathrm{a}}$, but ε_{a} is also a function of q_{v}, usually decreasing at high volume rates.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1741
Orange Book, p. 169

local flame temperature, T_1

in flame emission and absorption spectrometry

The effective thermodynamic temperature in the observation space as measured by a specific sensor for a specified element (in K). The temperature of a flame (or other plasma) is not homogeneous. It is usually lower at the borders of the flame. It is therefore appropriate to speak of an effective temperature which represents an average value of all temperatures throughout the observation space. The flame temperature depends on several factors such as: kind of plasma, kind of gas or gas mixture and concentration gradient of the thermometric species in the observation space.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1741

local fraction atomized, χ_a, β_a

in flame emission and absorption spectrometry

The substance fraction of the atomized component in the total volatilized component. This quantity is measured in a defined part of the flame, usually the observation space. The fraction atomized is the result of chemical reactions in the gaseous state. It depends on the bond strength of the compounds that the component may form within the flame and on the composition and temperature of the flame. When analysing elements that tend to become oxidized in the flame, it may be advisable to use as fuel gas mixtures with a reducing component such as C_2H_2 or N_2O .

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1741
Orange Book, p. 168

local fraction desolvated, χ_s, β_s

in flame emission and absorption spectrometry

The amount-of-substance fraction of component in a desolvated state in the amount of component entering the flame. This quantity is measured in a defined part of the flame, usually the observation space. Because it varies with height in the flame as a result of progressive evaporation of aerosol droplets, it is appropriate to term the expression local. The fraction desolvated does not account for losses by incomplete volatilization of the dry aerosol (which largely depends upon the nature and concentration of the component). Such losses are described by local fraction volatilized, which usually depends on the solute. Since χ_s varies markedly with the height in the flame, its observed value represents an average. Local fraction desolvated depends on the solvent, the temperature of the flame and the time the component takes to travel from the tip of the burner to the height in the flame considered.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1740
Orange Book, p. 168

local fraction volatilized, χ_v, β_v

in flame emission and absorption spectrometry

The substance fraction of the volatilized component in the total desolvated component. The gaseous state includes free atoms, molecules and radicals. This quantity is measured in a defined part of the flame, usually the observation space. The fraction volatilized varies inversely with the size of the desolvated particles. Since χ_v varies markedly with the height in the flame, its observed value represents an average.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1741
Orange Book, p. 168

localized adsorption

See: mobile adsorption, immobile adsorption

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

localized molecular orbitals (LMO)

The molecular orbitals located on certain fragments of a molecular system and spatially separated from each other as much as possible. The LMOs are derived from the electron occupied canonical molecular orbitals by subjecting them to a unitary transformation determined by an appropriate physical criterion, *e.g.* by maximizing the sum of squares of the centroids of occupied MOs (the Foster–Boys procedure) or by minimizing the sum of the exchange (or Coulomb) repulsion integrals between the occupied MOs (the Edmiston–Ruedenberg procedure).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1950

localized-itinerant transition

A transition of either of two types: (a) a Mott transition (single-valent systems). (b) a small-polaron to itinerant-electron transition (mixed-valent systems).

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 585

log-normal distribution

A distribution function $F(y)$, in which the logarithm of a quantity is normally distributed, i.e. $F(y) = f_{\text{gauss}}(\ln y)$ where $f_{\text{gauss}}(x)$ is a Gaussian distribution. The size distributions of atmospheric aerosols are often described using this distribution function, although the term also applies to gaseous pollutants.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

logarithmic normal distribution

of a macromolecular assembly

A continuous distribution with the differential mass-distribution function of the form:

$$f_{\text{w}}(x)\,\mathrm{d}x = \frac{1}{a\sqrt{\pi}\,x}\exp\left(-\frac{1}{a^2}\ln^2\frac{x}{b}\right)\mathrm{d}x$$

where x is a parameter characterizing the chain length, such as relative molecular mass or degree of polymerization and a and b are positive adjustable parameters.

Source:
Purple Book, p. 57

logit

In competitive binding assays, the logit-log dose relationship, in which the response is defined by: $R = \text{logit}(y) = \log_{10}\left(\frac{y}{1-y}\right)$ where $y = \frac{b}{b_0}$ with b = fraction of tracer bound and b_0 = value of b with no unlabelled ligand in the system. Logit transformed assay data frequently yield straight-line dose-response curves, amenable to statistical analysis.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

London forces

Synonym: dispersion forces

Attractive forces between apolar molecules, due to their mutual polarizability. They are also components of the forces between polar molecules. Also called 'dispersion forces'.
See also: van der Waals forces

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1136

London–Eyring–Polanyi (LEP) method

A semiempirical method of calculating a potential-energy surface, based on a simplified quantum-mechanical equation (the London equation).

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 171

London–Eyring–Polanyi–Sato (LEPS) method

A modification of the London–Eyring–Polanyi proposed in 1955 by S. Sato.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 171

lone (electron) pair

Two paired electrons localized in the valence shell on a single atom. Lone pairs should be designated with two dots. The term 'nonbonding electron pair' is more appropriate, and is found in many modern text books.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1137

long chain

A chain of high relative molecular mass.
See: macromolecule (1)

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2294

long spacing
in polymer crystals

The average separation between stacked lamellar crystals, usually measured by small-angle X-ray or neutron diffraction.

Source:
Purple Book, p. 82

long-lived collision complex

When a potential-energy surface is such that the system performs a number of vibrations and rotations in the region of a col, the corresponding intermediate is known as a long-lived collision complex, and the reaction is said to be indirect.

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 767

long-range intramolecular interaction

in polymers

An interaction between segments, widely separated in sequence along the chain, that occasionally approach one another during molecular flexing. This type of interaction is closely related to the excluded volume of a segment, the latter quantity reflecting interactions involving segments and solvent molecules. If no confusion can occur, the word 'intramolecular' may be omitted.

Source:
Purple Book, p. 48

longitudinal order

in a polymer

Order in the atomic positions along the chains of a linear polymer.

Source:
Purple Book, p. 46

loose end

Polymer chain within a network which is connected by a junction-point at one end only.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1820

Lorentz broadening [obsolete]

of a spectral line

See: collisional broadening *of a spectral line*

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1463

Lorentzian band shape

This band shape is described by the function:

$$F(\nu - \nu_0) = \frac{1}{\pi}\gamma\left((\nu - \nu_0)^2 + \gamma^2\right)^{-1}$$

where ν_0 is the mean band position, γ is the half band width at half maximum, and $F\,(\nu - \nu_0)$ is the frequency distribution function.
See also: Gaussian band shape

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2252

Lorenz–Mie theory

Theory of light scattering by isotropic, homogeneous spheres.

Source:
PAC, 1983, *55*, 931 *(Definitions, terminology and symbols in colloid and surface chemistry. Part 1.14: Light scattering (Provisional))* on page 935

lot

in analytical chemistry

A quantity of material which is assumed to be a single population for sampling purposes.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1201
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1463

low energy electron diffraction (LEED)

Any technique which measures the angular intensity distribution of electrons reflected from a crystalline surface under bombardment with low energy electrons ($E_0 < 500\ \mathrm{eV}$) in larger angles of incidence. The diffraction pattern also provides very surface sensitive information on the atomic arrangement of the top layers of a solid.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2025

low pressure electrical discharge

Low pressure electrical discharge sources are radiation sources in which radiation is produced by electrical discharges in gases at low pressures, i.e. pressures from 10^2 Pa to 10^{-3} Pa.

Source:
Orange Book, p. 145

low temperature UV–VIS absorption spectroscopy

The measurement of the absorption of UV–VIS radiation by a solute in a highly viscous or solid matrix at low temperature.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1452

low-pressure mercury lamp (arc)

Resonance lamp that contains mercury vapour at pressures of about $0.1\ \mathrm{Pa}$ (0.75×10^{-3} Torr; $1\ \mathrm{Torr} = 133.33\ \mathrm{Pa}$). At $25\ °\mathrm{C}$, such a lamp emits mainly at 253.7 and $184.9\ \mathrm{nm}$. They are also called germicidal lamps. There are cold- and hot-cathode as well as cooled electrode-less (excited by microwaves) low-pressure mercury lamps. The Wood lamp is a low-pressure mercury arc with an added fluorescent layer that emits in the *UV*-A spectral region (315–$400\ \mathrm{nm}$).

low-spin

Also contains definition of: high-spin

In any coordination entity with a particular d^n ($1<n<9$) configuration and a particular geometry, if the n electrons are distributed so that they occupy the lowest possible energy levels, the entity is a low-spin complex. If some of the higher energy d orbitals are occupied before all the lower energy ones are completely filled, then the entity is a high-spin complex.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1283

low-spin state

When the separation between the highest occupied and the lowest unoccupied molecular orbitals is not large, two alternative electronic states may be considered. The state with two electrons paired up in the HOMO is called a low-spin state. The low-spin state is the ground state when the one-electron energy needed to promote an electron to the LUMO is larger than the Coulomb and exchange repulsion energies required to pair up two electrons in the HOMO.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1950

lowest observed adverse effect level (LOAEL)

Lowest concentration or amount of a substance, found by experiment or observation, which causes an adverse alteration of morphology, functional capacity, growth, development, or life span of a target organism distinguishable from normal (control) organisms of the same species and strain under defined conditions of exposure.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2065
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1023
This definition replaces an earlier definition of .

lowest-observed-adverse-effect-level (LOAEL)

Lowest concentration or amount of a substance, found by experiment or observation, which causes an adverse alteration of morphology, functional capacity, growth, development, or life span of a target organism distinguishable from normal (control) organisms of the same species and strain under defined conditions of exposure.
See also: lowest-observed-effect-level, no-observed-adverse-effect-level, no-observed-effect-level,
This entry has been replaced by a new definition.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2065

lowest-observed-effect-level (LOEL)

Lowest concentration or amount of a substance, found by experiment or observation, that causes any alteration in morphology, functional capacity, growth, development, or life span of target organisms distinguishable from normal (control) organisms of the same species and strain under the same defined conditions of exposure.
See also: lowest-observed-adverse-effect-level, no-observed-adverse-effect-level, no-observed-effect-level

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2065

lumen

SI derived unit of luminous flux, $\mathrm{lm} = \mathrm{cd\ sr}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 979

luminance

Photometric counterpart of radiance, producing the visual sensation called brightness. Typical units are: candela m^{-2} (nit), candela cm^{-2} (stilb), foot lambert (2.426 nit). As with all photometric quantities, luminance does not refer to a specific wavelength, but applies to light emitted by a standard source (formerly a 'standard international candle', now a blackbody radiator emitting at the temperature of solidifying platinum, 2042 K). Conversion from photometric units to radiometric units (e.g. J s^{-1}) requires convolution over wavelength of the relative spectral response of the human eye (photopic response tables).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

luminescence

Spontaneous emission of radiation from an electronically or vibrationally excited species not in thermal equilibrium with its environment.
See also: bioluminescence, chemiluminescence, electro-generated chemiluminescence, fluorescence, phosphorescence, photoluminescence, radioluminescence, sonoluminescence, thermoluminescence, triboluminescence.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2252
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

See also:
Orange Book, p. 184
Orange Book, p. 231
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

luminescence quenching

Radiationless redistribution of excitation energy via interaction (electronic energy or charge transfer) between an emitting species and the quencher.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 235

luminescence spectrometer

The instrument used to measure luminescence emission spectra.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 238

luminous flux

Of a source of luminous intensity I in an element of solid angle $\mathrm{d}\Omega$ is given by $\mathrm{d}\Phi = I\,\mathrm{d}\Omega$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 979

luminous intensity I_v

Base quantity in the system of quantities upon which SI is based.

Source:
Green Book, 2nd ed., p. 4
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 979

luminous quantities

Group of quantities characterizing visible light in terms of the appearance to the human eye. The symbols of luminous quantities may be distinguished by adding a subscript v. The units for luminous quantities are derived from the SI base unit candela.
See also: radiant quantities, photon quantities

Source:
Green Book, 2nd ed., p. 30

lumiphore (luminophore)

A part of a molecular entity (or atom or group of atoms) in which electronic excitation associated with a given emission band is approximately localized. (Analogous to chromophore for absorption spectra).

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2253

lux

SI derived unit of illuminance, $\mathrm{lx} = \mathrm{lm\ m^{-2}} = \mathrm{cd\ sr\ m^{-2}}$.

Source:
Green Book, 2nd ed., p. 72

PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 979

lyases

Enzymes cleaving C–C, C–O, C–N and other bonds by other reactions than by hydrolysis or oxidation. Lyases catalyse the addition of molecules to unsaturated compounds or the elimination of molecules creating an unsaturated residue.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 159

lyate ion

The anion produced by hydron removal from a solvent molecule. For example, the hydroxide ion is the lyate ion of water.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1137

lyonium ion

The cation produced by hydronation of a solvent molecule. For example, (CH_3OH^{2+}) is the lyonium ion of methanol.
See also: onium compounds

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1137

lyophilic

Also contains definition of: lyophobic

The terms lyophilic (hydrophilic, lipophilic, oleophilic, etc.) and lyophobic (lipophobic, etc.) may be used to describe the character of interaction of a particular atomic group with the medium. In this usage the terms have the relative qualitative meaning of 'solvent preferring' (water-preferring, fat-preferring, etc.) and 'solvent rejecting' (water-rejecting, fat-rejecting, etc.) respectively.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

lyophilic sols

These comprise both association colloids in which aggregates of small molecules are formed reversibly and macromolecules in which the molecules themselves are of colloidal size.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

lyotropic mesophase

A mesophase formed by dissolving an amphiphilic mesogen in a suitable solvent, under appropriate conditions of concentration, temperature, and pressure.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 496

lysimeter

Laboratory column of selected representative soil or a protected monolith of undisturbed field soil with which it is possible to sample and monitor the movement of water and substances.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2065

μ- (mu)

in inorganic nomenclature

An affix used in names to signify that a group so designated bridges two or more centres of coordination.

Source:
Red Book, p. 245
Blue Book, p. 465

machine **[obsolete]**

in analysis

Usage not recommended.
See: analytical instrument

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1659

macrocycle

A cyclic macromolecule or a macromolecular cyclic portion of a macromolecule.
Notes:

1. ***See:*** chain (2)
2. In the literature, the term 'macrocycle' is sometimes used for molecules of low molecular mass that would not be considered 'macromolecules' as specified in the definition given in this book.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2298

macrolides

Macrocyclic lactones with a ring of twelve or more members.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

macrometeorology

in atmospheric chemistry

Study of the largest-scale aspects of the atmosphere, e.g. general global circulation.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

macromolecular isomorphism

Statistical co-crystallization of different constitutional repeating units which may either belong to the same copolymer chains (copolymer isomorphism) or originate from different homopolymer chains (homopolymer isomorphism). Isomorphism is a general term: in the strict sense, the crystal structure is essentially the same throughout the range of compositions; in isodimorphism or isopolymorphism, there are two or more crystal structures, respectively, depending on composition.

Source:
Purple Book, p. 80

macromolecule (polymer molecule)

Also contains definitions of: macromolecular, polymeric

A molecule of high relative molecular mass, the structure of which essentially comprises the multiple repetition of units derived, actually or conceptually, from molecules of low relative molecular mass.
Notes:

1. In many cases, especially for synthetic polymers, a molecule can be regarded as having a high relative molecular mass if the addition or removal of one or a few of the units has a negligible

effect on the molecular properties. This statement fails in the case of certain macromolecules for which the properties may be critically dependent on fine details of the molecular structure.
2. If a part or the whole of the molecule has a high relative molecular mass and essentially comprises the multiple repetition of units derived, actually or conceptually, from molecules of low relative molecular mass, it may be described as either macromolecular or polymeric, or by polymer used adjectivally.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2289

macromonomer

Polymer or oligomer the molecules of which each have one end-group that acts as a monomer molecule, so that each polymer or oligomer molecule contributes only a single monomer unit to a chain of the product polymer.
Notes:
1. The homopolymerization or copolymerization of a macromonomer yields a comb or graft polymer.
2. Macromonomers are also sometimes referred to as macromers. The use of the term 'macromer' is strongly discouraged.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 896

macromonomer molecule

A macromolecule that has one end-group which enables it to act as a monomer molecule, contributing only a single monomeric unit to a chain of the final macromolecule.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2290

macromonomeric unit (macromonomer unit)

The largest constitutional unit contributed by a single macromonomer molecule to the structure of a macromolecule.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2291

macropore

in catalysis

Pore with width exceeding about 0.05 μm or 50 nm (500 Å).

Cf. mesopore *in catalysis*, micropore *in catalysis*.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 585
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

macroporous polymer

Glass or rubbery polymer that includes a large number of macropores ($50\ \mathrm{nm}–1\ \mu\mathrm{m}$ in diameter) that persist when the polymer is immersed in solvents or in the dry state.
Notes:

1. Macroporous polymers are often network polymers produced in bead form. However, linear polymers can also be prepared in the form of macroporous polymer beads.
2. Macroporous polymers swell only slightly in solvents.
3. Macroporous polymers are used, for example, as precursors for ion-exchange polymers, as adsorbents, as supports for catalysts or reagents, and as stationary phases in size-exclusion chromatography columns.
4. Porous polymers with pore diameters from *ca* 2 to $50\ \mathrm{nm}$ are called mesoporous polymers.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 900

macroradical

A macromolecule which is also a free radical.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2290

macroscopic cross-section

The cross-section per unit volume of a given material for a specified process. For a pure nuclide, it is the product of the microscopic cross-section and the number of target nuclei per unit volume; for a mixture of nuclides, it is the sum of such products.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517
Orange Book, p. 218

macroscopic diffusion control [obsolete]

This terminology is not recommended.

See: mixing control

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 171

macroscopic film

A film which has lateral dimensions above $100\ \mu m$.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1671

macroscopic kinetics

A term applied to a kinetic study in which the interest is in the behaviour of bulk systems, e.g. in changes in concentrations of reactants and products.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 172

magic angle

Upon excitation of an 'isotropic' sample (assuming an ultra short excitation pulse) the relationship between the fluorescence intensity detected at a time t and through a polarization analyser oriented at an angle β with respect to the electric polarization of the exciting beam is given by

$$I(t,\ \beta) \propto N(t)\ [1 + (3\cos^2\beta - 1)\ R(t)]$$

where $R(t)$ is the degree of alignment of the emitting transition dipole in the laboratory frame and $N(t)$ is the excited-state population, both at time t. For $\beta = 54.7\ ^\circ$ (the magic angle), the dipole-alignment contribution vanishes and $I(t,\ \beta = 54.7\ ^\circ) \propto N(t)$.
Notes:

1. This concept also applies for time-resolved absorption measurements in cases in which photoselection occurs because the detected species do not freely rotate fast enough to make the measurement isotropic within the time of the experiment.
2. Applies for steady-state measurements on fixed samples. In this case

   $$I(\beta) \propto N\ [1 + (3\cos^2\beta - 1)\ R]$$

   with $I(\beta)$ the intensity of the effect observed at an analyser angle β with respect to the electric polarization of the exciting beam, N the excited-state population at steady-state equilibrium, and R the degree of alignment of the transition (dipole) moment of the excited molecular entity.
3. The term magic angle is also used in NMR spectroscopy.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 367

magnetic circular dichroism

Acronym: MCD

Magnetic circular dichroism is observed when a sample differentially absorbs left- and right-circularly polarized light in a magnetic field parallel to the light beam.
Notes:

1. The MCD signal, Δ, is calculated as

   $$\Delta = \frac{\alpha(\lambda)^{-} - \alpha(\lambda)^{+}}{\alpha(\lambda)^{-} + \alpha(\lambda)^{+}}$$

   with $\alpha(\lambda)^{-}$ and $\alpha(\lambda)^{+}$ the absorption coefficients for right and left circularly polarized light, respectively. The spectra are a representation of Δ vs wavelength. Often, Δ is recorded as a function of the applied field (up to $10\ \mathrm{T}$) and the temperature.
2. Phenomenon related to 'magnetically induced optical activity (Faraday effect)' by the 'Kramers-Kronig transformations', which connect optical refraction and absorption, i.e., MCD is observed in optically active materials at wavelengths with non-vanishing absorption. It occurs for diamagnetic, paramagnetic and (anti)-ferromagnetic material and has been observed from IR (infrared) to X-ray regions. MCD optical transitions in molecular species arise if (i) degenerate electronic states are split in the presence of a magnetic field (first-order-Zeeman effect) or (ii) states are mixed together by the applied magnetic field (second-order-Zeeman effect). This may occur in the initial or the final states.
3. MCD is used as a probe of paramagnetism that permits the identification of the electronic and magnetic properties of the ground states of transition metal ion centres. The wavelength dependence of MCD can be used also to identify and assign optical transitions from metal ion sites.
4. Technique complementary to both EPR and electronic absorption spectroscopies in facilitating assignment of the ground-state spin and electronic transitions of a molecular entity.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 368

magnetic deflection

in mass spectrometry

The deflection of an ion beam as a result of the motion of the ions in a magnetic field (magnetic sector). Generally the direction of motion of the ions is at right angles to the direction of the magnetic field, and the motion is uniform.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1544

Orange Book, p. 201

magnetic equivalence

Nuclei having the same resonance frequency in nuclear magnetic resonance spectroscopy and also identical spin-spin interactions with the nuclei of a neighbouring group are magnetically equivalent. The spin-spin interaction between magnetically equivalent nuclei does not appear, and thus has no effect on the multiplicity of the respective NMR signals. Magnetically equivalent nuclei are necessarily also chemically equivalent, but the reverse is not necessarily true.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1137

magnetic field (B) scan

in mass spectrometry

The usual method of producing a momentum (mass) spectrum, by varying the strength of the magnetic field.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

magnetic field strength, H

Magnetic flux density divided by the permeability.

Source:
Green Book, 2nd ed., p. 14

magnetic flux, Φ

Scalar product of magnetic flux density and area.

Source:
Green Book, 2nd ed., p. 14

magnetic flux density, $\boldsymbol{B}$

Also contains definition of: magnetic induction

Magnetic induction is a vector characterizing a magnetic field. The force acting on a moving charge in a magnetic field is the charge multiplied by the vector product of the velocity and magnetic flux density. This quantity is sometimes loosely called the magnetic field.
See also: flux

Source:
Green Book, 2nd ed., p. 14

magnetic flux density

in Mössbauer spectroscopy

Magnetic flux density at the nucleus (from experiment) in those cases in which the magnetic hyperfine interaction can be described by an effective field. In other cases the vector components of the magnetic hyperfine interaction should be reported if possible.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 214

magnetic moment, $\boldsymbol{m}$, $\boldsymbol{\mu}$

Vector quantity, the vector product of which with the magnetic flux density of a homogeneous field is equal to the torque.

Source:
Green Book, 2nd ed., p. 21

magnetic resonance imaging (MRI)

The visualisation of the distribution of nuclear spins (usually water) in a body by using a magnetic field gradient (NMR imaging). A similar technique, but less widely used, is to visualise the distribution of paramagnetic centres (EPR imaging).

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1284

magnetic susceptibility

For paramagnetic materials, the magnetic susceptibility may be measured experimentally and used to give information on the molecular magnetic dipole moment, and hence on the electronic structure of the molecules in the material. The paramagnetic contribution to the molar magnetic susceptibility of a material, χ, is related to the molecular magnetic dipole moment m by the Curie relation: $\chi = \frac{\text{constant x } m^2}{T}$.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1284

magnetic susceptibility, χ

Relative permeability minus one.

Source:
Green Book, 2nd ed., p. 15

magnetic transition

A transition between disordered and ordered arrays of atomic magnetic moments. Where the ordered phase has a net spontaneous magnetization, M_{S}, the magnetic-ordering temperature is called a Curie temperature, T_{C}; where the net spontaneous magnetization of the ordered phase remains zero, the ordering temperature is called a Néel temperature, T_{N}. The temperature at which the two ferromagnetic subarrays of a ferrimagnet just cancel each other is called the compensation point. Materials exhibit ferromagnetic behaviour when unpaired electron spins are aligned in parallel, antiferromagnetic behaviour when the alignment is antiparallel, and ferrimagnetic behaviour if the alignment of the spins is antiparallel with unequal numbers in the two orientations or if the spins are canted. Therefore, ferromagnetic, ferrimagnetic and weak ferromagnetic transitions involve a net magnetic moment change, whereas antiferromagnetic transitions have zero net magnetic moment change.
Note:
Antiferromagnetic order below T_{N} may be complex; for example, canting of spins as in $GdFeO_3$, spiral-spin configuration as may occur in MnO_2 , and amplitude modulation, as in some rare-earth metals.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 585

magnetizability, ξ

Tensor quantity relating the induced magnetic moment, $\boldsymbol{m}_{\mathrm{i}}$, to the applied magnetic flux density $\boldsymbol{B}$, $\boldsymbol{m}_{\mathrm{i}} = \xi\, \boldsymbol{B}$.

Source:
Green Book, 2nd ed., p. 21

magnetization transfer

NMR method for determining kinetics of chemical exchange by perturbing the magnetization of nuclei in a particular site or sites and following the rate at which magnetic equilibrium is restored. The most common perturbations are saturation and inversion, and the corresponding techniques are often called 'saturation transfer' and 'selective inversion-recovery'.
See also: saturation transfer

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1137

magnetogyric ratio, γ

Ratio of the magnetic moment to the angular momentum. It is often misleadingly called the gyromagnetic ratio.

Source:
Green Book, 2nd ed., p. 21

main chain (backbone)

of a polymer

That linear chain to which all other chains, long or short or both, may be regarded as being pendant.
Note:
Where two or more chains could equally be considered to be the main chain, that one is selected which leads to the simplest representation of the molecule.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2294

main-chain polymer liquid crystal

A polymer, whose molecules have mesogenic units only in their main chains.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 503

main-chain scission

Chemical reaction that results in the breaking of main-chain bonds of a polymer molecule.
Note:
Some main-chain scissions are classified according to the mechanism of the scission process: hydrolytic, mechano-chemical, thermal, photo-chemical, or oxidative scission. Others are classified according to their location in the backbone relative to a specific structural feature, for example, α-scission (a scission of the C–C bond alpha to the carbon atom of a photo-excited carbonyl group) and β-scission (a scission of the C–C bond beta to the carbon atom bearing a radical), etc.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 892

mancude-ring systems

Synonym: mancunide-ring systems

Rings having (formally) the maximum number of noncumulative double bonds, e.g. benzene, indene, indole, 4*H*-1,3-dioxine. Also called mancunide-ring systems.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

manipulator

A hand-operated or -controlled device for remotely handling radioactive materials.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

manual

in analysis

Refers to physical human intervention in an analytical procedure.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1659

mapping

in biotechnology

The determination of the relative positions of genes within the chromosomes of of restriction sites along a DNA molecule.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 159

Marangoni effect

Motions of the surface of a liquid are coupled with those of the subsurface fluid or fluids, so that movements of the liquid normally produce stresses in the surface and vice versa. The movement of the surface and of the entrained fluid(s) caused by surface tension gradients is called the Marangoni effect.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1218

Marcus equation (for electron transfer)

Relation between the rate of outer-sphere electron transfer and the thermodynamics of this process. Essentially, the rate constant within the encounter complex (or the rate constant of intramolecular transfer) is given by the Eyring equation:

$$k_{\mathrm{ET}} = \frac{\kappa_{\mathrm{ET}}\, k\, T}{h} \exp\left(-\frac{\Delta G^{\ddagger}}{R\, T}\right)$$

where k is the Boltzmann constant, h the Planck constant, R the gas constant and κ_{ET} the so-called electronic transmission factor ($\kappa_{\mathrm{ET}} \sim 1$ for adiabatic and $<< 1$ for diabatic electron transfer). For outer-sphere electron transfer the barrier height can be expressed as:

$$\Delta G^{\ddagger} = \frac{(\lambda + \Delta_{\mathrm{ET}} G^{\mathrm{o}})^2}{4\,\lambda}$$

where $\Delta_{\mathrm{ET}} G^{\mathrm{o}}$ is the standard Gibbs energy change accompanying the electron-transfer reaction and λ the total reorganization energy.
Note:
Whereas the classical Marcus equation has been found to be quite adequate in the normal region, it is now generally accepted that in the inverted region a more elaborate formulation, taking into account explicitly the Franck–Condon factor due to quantum mechanical vibration modes, should be employed.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 368

Marcus inverted region (for electron transfer)

See: inverted region

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2253

Marcus–Coltrin path

A path trajectory over a potential-energy surface which corresponds to the outermost vibrational turning points for the molecular species involved. This path was suggested as a device for calculating the probability of quantum-mechanical tunnelling: the trajectory for the system is considered to follow this path.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 172

Marcus–Hush relationship

Relationship between the barrier ($\Delta G^{\ddagger}$) to thermal electron transfer, the energy of a corresponding optical charge-transfer transition (ΔE_{op}), and the overall change in standard Gibbs energy accompanying thermal electron transfer (ΔG^{o}). Assuming a quadratic relation between the energy of the system and its distortions from equilibrium (harmonic oscillator model) the expression obtained is:

$$\Delta G^{\ddagger} = \frac{{\Delta E_{\mathrm{op}}}^{2}}{4\,(\Delta E_{\mathrm{op}} - \Delta G^{\mathrm{o}})}$$

The simplest form of this expression obtains for degenerate electron transfer (ΔG^{o}) in e.g. symmetrical mixed valence systems:

$$\Delta G^{\ddagger} = \frac{\Delta E_{\mathrm{op}}}{4}$$

Note that for this situation the Marcus equation reads:

$$\Delta G^{\ddagger} = \frac{\lambda}{4}$$

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2253

marker

1. (DNA) A fragment of known size used as reference for analytical purposes.
2. (genetic) A gene with known phenotype and mapped position.
3. (chromatography) A reference substance co-chromatographed with the sample to assist in identifying the components.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 159
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 837
Orange Book, p. 97

Markownikoff rule

Also contains definition of: anti-Markownikoff addition

'In the addition of hydrogen halides to unsymmetrically constituted [unsaturated] hydrocarbons, the halogen atom becomes attached to the carbon bearing the lesser number of hydrogen atoms.' Originally formulated by Markownikoff (Markovnikov) to generalize the orientation in additions of hydrogen halides to simple alkenes, this rule has been extended to polar addition reactions as follows. 'In the heterolytic addition of a polar molecule to an alkene or alkyne, the more electronegative (nucleophilic) atom (or part) of the polar molecule becomes attached to the carbon atom bearing the smaller number of hydrogen atoms.' This is an indirect statement of the common mechanistic observation, that the more electropositive (electrophilic) atom (or part) of the polar molecule becomes attached to the end of the multiple bond that would result in the more stable carbenium ion (whether or not a carbenium ion is actually formed as a reaction intermediate in the addition reaction). Addition in the opposite sense is commonly called 'anti-Markovnikov addition'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1137

Mark–Houwink equation

The equation describing the dependence of the intrinsic viscosity of a polymer on its relative molecular mass (molecular weight) and having the form:

$$[\eta] = K{\cdot}M_{\mathrm{r}}^{a}$$

where $[\eta]$ is the intrinsic viscosity, K and a are constants the values of which depend on the nature of the polymer and solvent as well as on temperature and M_{r} is usually one of the relative molecular mass averages.
Notes:

1. The use of this equation with the relative molecular mass (molecular weight) is recommended, rather than with molar mass (which has the dimension of mass divided by amount of substance), since in the latter case the constant K assumes awkward and variable dimensions owing to the fractional and variable nature of the exponent a.
2. Kuhn and Sakurada have also made important contributions and their names are sometimes included, as, for example, in the Kuhn–Mark–Houwink–Sakurada equation.

Source:
Purple Book, p. 64

martensitic transition

A diffusionless transition (first studied in the steel alloy, Martensite), at constant composition, generated by coordinated atomic, ionic or molecular displacements over distances smaller than interatomic distances in the parent phase. The cooperative rearrangements of the crystal structure generally take place progressively by the movement of a two-dimensional interface through the solid. Examples: The face-centred-cubic to body-centred-tetragonal transition of iron containing some carbon; the transition of tetragonal ZrO_2 to monoclinic ZrO_2 .

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 585

mass, *m*

Base quantity in the system of quantities upon which SI is based.

Source:
Green Book, 2nd ed., p. 12

PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 979

mass analysis

in mass spectrometry

A process by which a mixture of ionic or neutral species is identified according to the mass-to-charge ($\frac{m}{z}$) ratios (ions) or their aggregate atomic masses (neutrals). The analysis may be qualitative and/or quantitative.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545

mass balance

in atmospheric chemistry

Summation of the masses of a given element in its various compounds before and after reaction (changes) in the atmosphere; provides a test of the completeness of the accounting of the various reaction paths for this element which can be had through the compounds which have been analysed.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

mass concentration, γ, ρ

Mass of a constituent divided by the volume of the mixture.
See: concentration

Source:
Green Book, 2nd ed., p. 42
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 979

mass density

See: density

Source:
Green Book, 2nd ed., p. 12

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 980

mass density gradient, $\nabla\rho$, grad ρ

Change in mass density in a small distance divided by that distance.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 980

mass distribution ratio

in chromatography

The fraction $(1 - R)$ of a component in the stationary phase divided by the fraction (R) in the mobile phase:

$$D_{\mathrm{m}} = \frac{\text{amount of substance in the stationary phase}}{\text{amount of component in the mobile phase}}$$

This term is recommended in preference to the term capacity factor frequently used in the chromatographic literature.
See also: extraction factor

Source:
Orange Book, p. 107
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2384

mass distribution ratio, k_{MEKC}

in micellar electrokinetic chromatography

Defined as:

$$k_{\mathrm{MEKC}} = \frac{n_{\mathrm{mc}}}{n_{\mathrm{aq}}} = K \cdot \frac{V_{\mathrm{mc}}}{V_{\mathrm{aq}}}$$

where n_{mc} and n_{aq} are the chemical amounts of the analyte in the micellar and aqueous phases, respectively, K is the distribution constant and V_{mc} and V_{aq} are the corresponding volumes of the phases.
Notes:

1. In the case of an electrically neutral analyte, k_{MEKC} can be calculated directly from the migration times:

   $$k_{\mathrm{MEKC}} = \frac{t_{\mathrm{m}} - t_{\mathrm{eo}}}{t_{\mathrm{eo}}} \left(1 - \frac{t_{\mathrm{m}}}{t_{\mathrm{mc}}}\right)$$

2. k_{MEKC} should not be confused with the retention factor (in column chromatography) k. However, k_{MEKC} is analogous to the mass distribution ratio (in chromatography).

Source:
PAC, 2004, *76*, 443 *(Terminology for analytical capillary electromigration techniques (IUPAC Recommendations 2003))* on page 449

mass distribution ratio, k_{MEEKC}

in micro-emulsion electrokinetic chromatography

Defined analogously to mass distribution ratio (in micellar electrokinetic chromatography), k_{MEEKC} by replacing terms for micelles with corresponding terms for micro-emulsion.

Source:
PAC, 2004, *76*, 443 *(Terminology for analytical capillary electromigration techniques (IUPAC Recommendations 2003))* on page 449

mass excess, Δ

Mass of an atom minus the product of mass number and atomic mass constant.

Source:
Green Book, 2nd ed., p. 20

mass flow rate, q_{m}

Mass of a material crossing a surface divided by the time.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 980

mass fraction, w

Mass of a constituent divided by the total mass of all constituents in the mixture.

Source:
Green Book, 2nd ed., p. 41
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 980

mass number, A

Total number of heavy particles (protons and neutrons jointly called nucleons) in the atomic nucleus. Also called nucleon number. Symbol m in mass spectrometry.

Source:
Green Book, 2nd ed., p. 20
Red Book, p. 35

PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 980
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545

mass peak

in mass spectrometry

A record of the ion current, at a specific mass to charge ratio, received by the collector.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

mass range

in mass spectrometry

The range of mass numbers which can be characterized by a mass spectrometer with sufficient resolution to differentiate adjacent peaks.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

mass resolving power

in mass spectrometry

Commonly and also acceptably defined in terms of the overlap (or 'valley') between two peaks. Thus for two peaks of equal height, masses m_1 and m_2, when there is overlap between the two peaks to a stated percentage of either peak height (10% is recommended), then the resolving power is defined as $\frac{m_1}{m_1 - m_2}$. The percentage overlap (or 'valley') concerned must always be stated.

Source:
PAC, 1978, *50*, 65 *(Recommendations for symbolism and nomenclature for mass spectroscopy)* on page 72

mass spectrograph

An instrument in which beams of ions are separated (analysed) according to the quotient mass/charge, and in which the deflection and intensity of the beams are recorded directly on photographic plate or film.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545

mass spectrometer

An instrument in which beams of ions are separated (analysed) according to the quotient mass/charge, and in which the ions are measured electrically. This term should also be used when a scintillation detector is employed.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545
Orange Book, p. 201

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

mass spectrometer focusing system (deflection system)

An assembly permitting the separation of ions according to their mass-to-charge ratio.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

mass spectrometer (operating on the linear accelerator principle)

A mass spectrometer in which the ions to be separated absorb maximum energy through the effect of alternating electric fields which are parallel to the path of the ions. These ions are then separated from other ions with different mass/charge by an additional electric field.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545

mass spectrometric detector
in gas chromatography

A mass spectrometer used as a detector to give qualitative and quantitative data on the various eluted substances. The mass spectrum of the eluted compounds provides evidence beyond the elution time as to the chemical nature of the species.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

mass spectrometry

The branch of science dealing with all aspects of mass spectroscopes and the results obtained with these instruments.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546
Orange Book, p. 201

mass spectroscope [obsolete]

A term (now essentially obsolete) which may refer to either a mass spectrometer or a mass spectrograph.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

mass spectroscopy

The study of systems by causing the formation of gaseous ions, with or without fragmentation, which are then characterized by their mass-to-charge ratios and relative abundances.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

mass spectrum

A spectrum which is obtained when a beam of ions is separated according to the mass-to-charge ($\frac{m}{z}$) ratios of the ionic species contained within it.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

See also:
Orange Book, p. 204
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

mass transfer coefficient

in electrochemistry

The heterogeneous diffusion rate constant defined for the case of the limiting current. A more general definition in terms of the electrode current densities is:

$$k_{\mathrm{d}} = \frac{j\,\nu}{n\,F\,(c_{\mathrm{e}} - c_{0})}$$

or

$$k_{\mathrm{d}} = \frac{j\,\nu\,(1 - t_{\mathrm{B}}\,n\,\nu^{-1}\,z_{\mathrm{B}}{}^{-1})}{n\,F\,(c_{\mathrm{e}} - c_{0})}$$

where j is the electrode current density, ν is the stoichiometric number, n is the charge number of the electrode reaction, F is the Faraday constant, c_{e} is the interfacial concentration, c_0 is the bulk concentration, t_{B} is the transport number of species B, and z_{B} is the charge number of species B.

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1839

mass transfer

in biotechnology

Spontaneous (irreversible) process of transfer of mass across non-homogeneous fields. The driving force can be difference in concentration (in liquids) or partial pressure (in gases) of the component. In fluids, mass transfer may be enhanced by turbulent flow. In biological systems, mass transfer through membranes may result from normal diffusion, facilitated diffusion or active transport.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 159

mass (weight) of the stationary phase, W_{s}

in chromatography

The mass (weight) of the liquid stationary phase or the active solid in the column. The mass (weight) of any solid support is not included. In the case of partition chromatography with a liquid stationary phase it is identical to the liquid phase mass (weight).

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 833

mass-average velocity

Also contains definition of: molar average velocity *in electrolytes*

in electrolytes

Mass-average velocity:

$$v_b = \rho^{-1} \sum C_i M_i v_i$$

Cf. molar average velocity:

$$v_m = c_t^{-1} \sum c_i v_i$$

with $c_t = \sum c_i$ where M_i = molar mass, c_t = total concentration (mol m^{-1}), ρ = density of the solution (kg m^{-3}).

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1831

mass-distribution function

Synonym: weight-distribution function

A distribution function in which the relative amount of a portion of a substance with a specific value, or a weight distribution range of values, of the random variable(s) is expressed in terms of mass fraction.

Source:
Purple Book, p. 56

mass-flow sensitive detector

in chromatography

A device the response of which is proportional to the amount of sample component reaching the detector in unit time.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 849

mass-law effect

At equilibrium, the product of the activities (or concentrations) of the reacting species is constant. Thus for the equilibrium:

$$\alpha \mathrm{A} + \beta \mathrm{B} \rightleftharpoons \gamma \mathrm{C} + \delta \mathrm{D}$$

$$K = \frac{[\mathrm{C}]^{\gamma}\,[\mathrm{D}]^{\delta}}{[\mathrm{A}]^{\alpha}\,[\mathrm{B}]^{\beta}}$$

See also: common-ion effect, equilibrium

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1138

mass-to-charge ratio, $\frac{m}{z}$

in mass spectrometry

The abbreviation $\frac{m}{z}$ is used to denote the dimensionless quantity formed by dividing the mass number of an ion by its charge number. It has long been called the mass-to-charge ratio although m is not the ionic mass nor is z a multiple or the elementary (electronic) charge, e. The abbreviation $\frac{m}{e}$ is, therefore, not recommended. Thus, for example, for the ion ($C_7H_7^{2+}$) , $\frac{m}{z}$ equals 45.5.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1544

mass-transfer-controlled electrolyte rate constant

In controlled-potential coulometry and related techniques, the empirically evaluated constant of proportionality defined by the equation

$$s_{\mathrm{B}} = -\frac{1}{c_{\mathrm{B}}}\frac{\mathrm{d}c_{\mathrm{B}}}{\mathrm{d}t}$$

where c_{B} is the bulk concentration of the substance B, and $\frac{\mathrm{d}c_{\mathrm{B}}}{\mathrm{d}t}$ is the rate of change of that concentration, resulting from the consumption of B by reduction or oxidation at the working electrode.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1501

massic

Attribute to a physical quantity obtained by division by mass; synonymous with specific.

Source:
ISO 31-0: 1992 *(Quantities and Units - Part 0: General Principles, Units and Symbols.)*
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 980

massive transition

A transition in which a crystal structure is changed into a new structure during cooling or heating, predominantly by interface-controlled reactions and the usual nucleation and growth characteristics associated with thermal diffusion.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 585

matched cells

Also contains definition of: reference cell (or blank cell) *in spectrochemical analysis*

in spectrochemical analysis

A pair of cells with closely similar optical properties are called matched cells. One cell is the sample cell while the other, the reference (or blank) cell contains the solvent or a reference solution. In double beam spectrometers, radiation is passed either simultaneously or alternately through the cells. In single beam instruments the cells are moved sequentially into the radiation beam.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1453

material safety data sheet (MSDS)

Compilation of information required under the US OSHA Hazard Communication Standard on the identity of hazardous substances, health and physical hazards, exposure limits and precautions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2066

matrix effect

1. (*in analytical chemistry*) The combined effect of all components of the sample other than the analyte on the measurement of the quantity. If a specific component can be identified as causing an effect then this is referred to as interference.
   See: matrix

   Source:
   PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660
2. (*in surface analysis*) Effects which cause changes in Auger-electron, photoelectron, secondary ion yield, or scattered ion intensity, the energy or shape of the signal of an element in any environment as compared to these quantities in a pure element. (a) Chemical matrix effects: changes in the chemical composition of the solid which affect the signals as described above. (b) Physical matrix effects: topographical and/or crystalline properties which affect the signal as described above.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

matrix

in analysis

The components of the sample other than the analyte.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

matrix isolation

A term which refers to the isolation of a reactive or unstable species by dilution in an inert matrix (argon, nitrogen, etc.), usually condensed on a window or in an optical cell at low temperature, to preserve its structure for identification by spectroscopic or other means.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1138
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

Mattauch–Herzog geometry

An arrangement for a double-focusing mass spectrograph in which a deflection of $\frac{\pi}{4\sqrt{2}}$ radians in a radial electrostatic field is followed by a magnetic deflection of $\frac{\pi}{2}$ radians.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

maximum allowable concentration

in atmospheric chemistry

The maximum concentration of a pollutant which is considered harmless to healthy adults during their working hours, assuming they breathe uncontaminated air at all other times.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

See also:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2066

maximum emission concentration

in atmospheric chemistry

Standards for maximum concentration of air pollutant emission from stationary or mobile sources.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2200

maximum hardness, principle of

A chemical system at a given temperature will evolve to a configuration of maximum absolute hardness, η, provided that the potential due to the nuclei, plus any external potential and the electronic chemical potential, remain constant. In terms of molecular orbital theory, the highest value of η reflects the highest possible energy gap between the lowest unoccupied and highest occupied molecular orbitals; this value correlates with the stability (***See:*** structural stability; electronic stability) of a system.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1950

maximum latent period

The length of time after which no causal relationship can reasonably be established. This length of time is the period from the last exposure to the point of time at which an exposed person has demonstrated the initial signs or symptoms.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1023

maximum permissible daily dose

Maximum daily dose of substance whose penetration into a human body during a lifetime will not cause diseases or health hazards that can be detected by current investigation methods and will not adversely affect future generations.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2067

maximum permissible level (MPL)

Level, usually a combination of time and concentration, beyond which any exposure of humans to a chemical or physical agent in their immediate environment is unsafe.
See also: maximum allowable concentration

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2067

maximum storage life

Period during which there is no change in concentration in excess of the value of the uncertainty of the concentration.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2201

maximum tolerable concentration (MTC)

Highest concentration of a substance in an environmental medium that does not cause death of test organisms or species (denoted by LC_0).

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2067

maximum tolerable dose (MTD)

Highest amount of a substance that, when introduced into the body, does not kill test animals (denoted by LD_0).

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2067

maximum tolerable exposure level (MTEL)

Maximum amount or concentration of a substance to which an organism can be exposed without leading to an adverse effect after prolonged exposure time.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2068

maximum tolerated dose (MTD)

High dose used in chronic toxicity testing that is expected on the basis of an adequate subchronic study to produce limited toxicity when administered for the duration of the test period. It should not induce: (a) overt toxicity, for example appreciable death of cells or organ dysfunction, or (b) toxic manifestations that are predicted materially to reduce the life span of the animals except as the result of neoplastic development or (c) 10% or greater retardation of body weight gain as compared with control animals. In some studies, toxicity that could interfere with a carcinogenic effect is specifically excluded from consideration.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2068

McLafferty rearrangement

in mass spectrometry

β-Cleavage with concomitant specific transfer of a γ-hydrogen atom in a six-membered transition state in mono-unsaturated systems, irrespective of whether the rearrangement is formulated by a radical or an ionic mechanism, and irrespective of the position of the charge.

Source:
Orange Book, p. 207

mean activity of an electrolyte in solution

Defined by the equation:

$$a_{\pm} = \mathrm{e}^{(\mu_{\mathrm{B}} - \mu_{\mathrm{B}}^{\ominus})\, \nu\, R\, T}$$

where μ_{B} is the chemical potential of the solute B in a solution containing B and other species. The nature of B must be clearly stated: it is taken as a group of ions of two kinds carrying an equal number of positive and negative charges, e.g. $\mathrm{Na}^{+} + \mathrm{NO_3}^{-}$ or $\mathrm{Ba}^{2+} + 2\mathrm{Cl}^{-}$ or $2\mathrm{Al}^{3+} + 3\mathrm{SO_4}^{2-}$. ν is the total number of ions making up the group i.e. 2, 3 and 5 respectively in the above examples. $\mu_{\mathrm{B}}^{\ominus}$ is the chemical potential of B in its standard state, usually the hypothetical ideal solution of concentration $1\ \mathrm{mol\ kg^{-1}}$ and at the same temperature and pressure as the solution under consideration.
See also: activity

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 510

mean (average), $\bar{x}$

The sum of a series of observations divided by the number of observations in the series.

Source:
Orange Book, p. 4

mean catalytic activity rate, $\frac{\Delta z}{\Delta t}$

The catalytic activity of a specified component in or moved from a system divided by the time during which the component was changed or moved. This kind of quantity should not be confused with rate of reaction.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2475

mean current density

Defined as

$$j = \frac{I}{A}$$

where I is the electric current and A is usually taken as the geometric area of the electrode. However the nature of the area used in this calculation must be clearly stated. In interpreting the mean current density it is important to know whether the current is uniformly distributed over the electrode interface.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 513

mean exchange current density

Defined by

$$j_0 = \frac{I_0}{A}$$

where I_0 is the exchange current of the electrode reaction and A is usually taken as the geometric area of the electrode.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 516

mean free path, λ

The average distance a molecule travels between collisions. For a molecule, $\lambda = (\sqrt{2}\ \pi\ n\ {d_\mathrm{m}}^2)^{-1}$, where n is the number of molecules per unit volume and d_m is their mean diameter. For O_2 at one atmosphere and $25\ °\mathrm{C}$, this distance is only $9.7 \times 10^{-6}\ \mathrm{cm}$; at 10^{-6} atmospheres and $25\ °\mathrm{C}$ it is $9.7\ \mathrm{cm}$. For an aerosol particle, the mean free path, λ_B in the Stokes region (see Stokes law) is given by: $\lambda_\mathrm{B} = \sqrt{\frac{3\,k\,T}{m}}\ m\,B$ where m is the mass of the particle, k is the Boltzmann constant $(1.381 \times 10^{-23}\ \mathrm{J\ K^{-1}})$, T is the temperature (K) and B is the mobility.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2201
Green Book, 2nd ed., p. 56

mean interstitial velocity of the carrier gas

in chromatography

The interstitial velocity, u of the carrier gas multiplied by the pressure-gradient correction-factor, j:

$$\bar{u} = u\ j$$

$$\bar{u} = \frac{F\ j}{\varepsilon_\mathrm{I}}$$

where F is the nominal linear flow, ε_I is the interstitial fraction.

Source:
Orange Book, p. 103

mean life, τ

See: lifetime

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1138

mean linear range

in nuclear chemistry

In a given material, for specified charged particles of a specified energy, the average displacement of the particles before they stop.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

mean mass range

in nuclear chemistry

The mean linear range multiplied by the mass density of the material.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

mean mass rate, $\frac{\Delta m}{\Delta t}$

The mass of a specified component changed in or moved to or from a system divided by the time during which the component was changed or moved.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2474

mean residence time

of adsorbed molecules

The mean time during which the molecules remain on the surface of the adsorbent, i.e. the mean time interval between impact and desorption.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

mean substance rate, $\frac{\Delta n}{\Delta t}$

The amount of substance of a specified component changed in or moved to or from a system divided by the time during which the component was changed or moved. This kind of quantity usually should be preferred to mean mass rate or mean volume rate.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2475

mean volume rate, $\frac{\Delta V}{\Delta t}$

The volume of a specified component changed in or moved to or from a system divided by the time during which the component was changed or moved.
See also: clearance

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2474
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 980

measurable quantity

An attribute of a substance which may be distinguished qualitatively and determined quantitatively. In the context of analytical chemistry, the attribute may refer to a physical quantity such as X- or γ-ray energy, or it may refer to a measure of amount such as mass or concentration.

Source:
VIM
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1701

measurand

Particular quantity subject to measurement.

Source:
VIM
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 980

measured excitation spectrum

The spectrum observed by measuring the variation of the luminescence flux from an analyte as a function of the excitation wavelength.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 242

measured spectrum

Synonymous with spectrogram.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

measured value

in analysis

The observed value of weight, volume, meter-reading or other quantity, found in the analysis of a material.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 597

measurement

A description of a property of a system by means of a set of specified rules, that maps the property onto a scale of specified values, by direct or 'mathematical' comparison with specified reference(s). The demand for rules makes 'measurement' a scientific concept in contrast to the mere colloquial sense of 'description'. However, in the present definition, 'measurement' has a wider meaning than given in elementary physics. Even a very incomplete description of, for instance, a patient (at a stated time) has to be given by a set of measurements, that are easier to manage and grasp.

Source:
PAC, 1995, *67*, 1563 *(Properties and units in the clinical laboratory sciences-I. Syntax and semantic rules (IUPAC-IFCC Recommendations 1995))* on page 1565

measurement resolution

in atmospheric trace component analysis

The minimum value above which the difference of two values of air quality characteristic can be distinguished with 95% probability.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2201

measurement result

Also contains definitions of: bias, expectation value, expected value, limiting mean

The outcome of an analytical measurement (application of the chemical measurement process), or value attributed to a measurand. This may be the result of direct observation, but more commonly it is given as a statistical estimate derived from a set of observations. The distribution of such estimates (estimator distribution) characterizes the chemical measurement process, in contrast to a particular estimate, which constitutes an experimental result. Additional characteristics become evident if we represent $\hat{x}$ as follows:

$$\hat{x} = \tau + e = \underbrace{\tau + \mathrlap{\overbrace{}^{e}}\Delta}_{\mu} + \delta = \mu + \delta$$

The true value, τ, is the value x that would result if the chemical measurement process were error-free. The error, e, is the difference between an observed (estimated) value and the true value; i.e. $e = \hat{x} - \tau$ (signed quantity). The total error generally has two components, bias (Δ) and random error (δ), as indicated above. The limiting mean, μ, is the asymptotic value or population mean of the distribution that characterizes the measured quantity; the value that is approached as the number of observations approaches infinity. Modern statistical terminology labels this quantity the expectation value or expected value, $E(\hat{x})$. The bias, Δ, is the difference between the limiting mean and the true value; i.e. $\Delta = \mu - \tau$ (signed quantity). The random error, δ, is the difference between an observed value and the limiting mean; i.e. $\delta = \hat{x} - \mu$ (signed quantity).

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1705

measurement solution

in analysis

The solution that is presented to the measuring device. It comprises the test solution, or an aliquot thereof, after it has undergone any treatment required prior to the presentation to the measuring device.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

measurement threshold

of an analyser

The minimum concentration of a substance which produces a quantifiable signal with a given uncertainty.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

mechanical entrapment

1. The process of random incorporation of comparatively small quantities of other phases (e.g. water, dust, particles, etc.) in the bulk of a precipitate during its formation.

2. The deliberate capture of small quantities of such phases by the deliberate addition of solids to a liquid phase. (The term inclusion is not recommended).

Source:
Orange Book, p. 85

mechanical hygrometer

An apparatus containing an element (hair, goldbeater's skin, carbon-film) whose dimension or mass varies as a function of its water content.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2195

mechanism

Synonym: reaction mechanism

of a reaction

A detailed description of the process leading from the reactants to the products of a reaction, including a characterization as complete as possible of the composition, structure, energy and other properties of reaction intermediates, products and transition states. An acceptable mechanism of a specified reaction (and there may be a number of such alternative mechanisms not excluded by the evidence) must be consistent with the reaction stoichiometry, the rate law and with all other available experimental data, such as the stereochemical course of the reaction. Inferences concerning the electronic motions which dynamically interconvert successive species along the reaction path (as represented by curved arrows, for example) are often included in the description of a mechanism. It should be noted that for many reactions all this information is not available and the suggested mechanism is based on incomplete experimental data. It is not appropriate to use the term mechanism to describe a statement of the probable sequence in a set of stepwise reactions. That should be referred to as a reaction sequence, and not a mechanism.
See also: Gibbs energy diagram

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1138

mechanism-based inhibition

Synonym: suicide inhibition

Irreversible inhibition of an enzyme due to its catalysis of the reaction of an artificial substrate. Also called 'suicide inhibition'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1138

mechanization

in analysis

The use of devices to replace, refine, extend or supplement human effort. The corresponding verb is to mechanize.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1659

Mechano-chemical reaction

Chemical reaction that is induced by the direct absorption of mechanical energy.
Note:
Shearing, stretching, and grinding are typical methods for the mechano-chemical generation of reactive sites, usually macroradicals, in polymer chains that undergo mechano-chemical reactions.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 893

median

Depending on whether the number of observations is even or odd, the median can be estimated as follows:

1. If $n = 2\,m + 1$: The middle value of a series of observations, arranged in increasing or decreasing order.
2. If $n = 2\,m$: The arithmetic mean of the two middle values of a series of observations, arranged in increasing or decreasing order.

Comment: The use of the median when reporting results of chemical analysis is generally not recommended, because its statistical efficiency is less than that of the mean. In certain cases, however, especially when treating small sets of data, the median may offer advantages because it is a so-called 'robust statistic', i.e. it offers considerable resistance to the effects of isolated outliers.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 603

median effective concentration (EC_{50})

Statistically derived concentration of a substance in an environmental medium expected to produce a certain effect in 50% of test organisms in a given population under a defined set of conditions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2068

median effective dose (ED_{50})

Statistically derived dose of a chemical or physical agent (radiation) expected to produce a certain effect in 50% of test organisms in a given population or to produce a half-maximal effect in a biological system under a defined set of conditions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2068

median lethal concentration (LC_{50})

Statistically derived concentration of a substance in an environmental medium expected to kill 50% of organisms in a given population under a defined set of conditions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2068

median lethal dose (LD_{50})

Statistically derived dose of a chemical or physical agent (radiation) expected to kill 50% of organisms in a given population under a defined set of conditions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2068

median lethal time (TL_{50})

Statistically derived average time interval during which 50% of a given population may be expected to die following acute administration of a chemical or physical agent (radiation) at a given concentration under a defined set of conditions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2068

median narcotic concentration (NC_{50})

Statistically derived concentration of a substance in an environmental medium expected to cause narcotic conditions in 50% of a given population under a defined set of conditions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2068

median narcotic dose (ND_{50})

Statistically derived dose of a substance expected to cause narcosis in 50% of test animals under a defined set of conditions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2068

medium

The phase (and composition of the phase) in which chemical species and their reactions are studied in a particular investigation.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1138

medium effect

The medium effect on ionic species B due to transfer from solvent S_1 to solvent S_2 (number) is defined by

$$R\,T\,\ln \gamma_{\mathrm{S}_1}^{\mathrm{S}_2}(\mathrm{B}) = \mu_{\mathrm{B}}^{\mathrm{o},\mathrm{S}_2} - \mu_{\mathrm{B}}^{\mathrm{o},\mathrm{S}_1}$$

where R is the gas constant, T is the thermodynamic temperature and $\mu_{\mathrm{B}}^{\mathrm{o},\mathrm{S}_i}$ is the standard chemical potential of B in solvent S_i (where $i = 1$ or 2), the reference states being the same in both solvents. $\gamma_{\mathrm{S}_1}^{\mathrm{S}_2}(\mathrm{B})$ is not an exactly measurable quantity.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 508

medium-pressure mercury lamp

Also contains definition of: medium-pressure mercury arc

Non-coherent radiation source containing mercury vapour at pressures ranging from 50 to several hundred kPa (1 atm = 101.325 kPa). Emits mostly from 200 to 1000 nm with the most intense lines approximately at 218, 248, 254, 266, 280, 289, 297, 303, 313, 334, 366, 406, 408, 436, 546 and 578 nm.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 369

mega

SI prefix for 10^6 (symbol: M).

Source:
Green Book, 2nd ed., p. 74

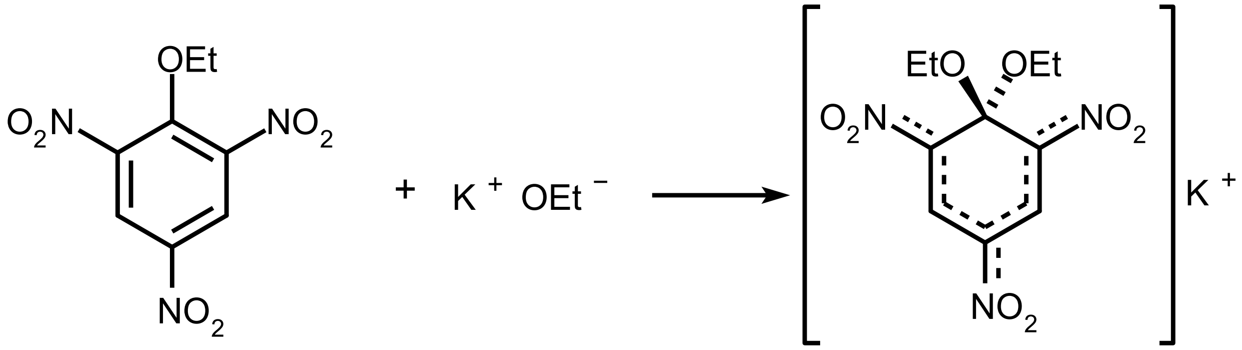
meiosis

The reductive cell division which results in daughter cells containing one copy of each of the chromosomes of the parent. The entire meiotic process involves two separate divisions (meiosis I and meiosis II). The first division is a true reductive division with the chromosome number being halved, whereas the second division resembles mitosis in many ways. Thus, a diploid parental cell will give rise to haploid daughter cells (cf. ploidy).

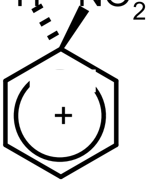
Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 159

Meisenheimer adduct

A cyclohexadienyl derivative formed as Lewis adduct from a nucleophile (Lewis base) and an aromatic or heteroaromatic compound, also called Jackson–Meisenheimer adduct. In earlier usage the term 'Meisenheimer complex' was restricted to the typical Meisenheimer alkoxide adducts of nitro-substituted aromatic ethers, e.g.



Analogous cationic adducts, such as:



considered to be reaction intermediates in electrophilic aromatic substitution reactions, are called 'Wheland intermediates', and sometimes, inappropriately, σ-complexes.
See also: σ-adduct

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1138

See also:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

melting

The conversion of a solid to a liquid by the application of heat and/or pressure.
Note:
For a liquid crystal, melting occurs when the three-dimensional periodic structure of a solid collapses to give a liquid-crystal phase in which the molecules have orientational order, but not long range translational order.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 585

melting point (corrected/uncorrected)

The term originally signified that a correction was made (not made) for the emergent stem of the thermometer. In current usage it often means that the accuracy of the thermometer was (was not) verified. This current usage is inappropriate and should be abandoned.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1139

membrane

Structure, having lateral dimensions much greater than its thickness, through which transfer may occur under a variety of driving forces.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1482

membrane emf

The potential difference E_m between two saturated KCl bridges inserted into two solutions separated by a membrane. The solutions need not be in equilibrium with one another and need not contain any colloidal material.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 619

membrane

in an ion-selective electrode

A general term which refers to a continuous layer, usually consisting of a semi-permeable material, with controlled permeability covering a structure, such as carbon or an inert metal, or separating two electrolyte solutions. This latter case is the most general form of an ion-selective electrode. The membrane separates the internal components of the ion-selective electrode from the test solution. The membrane of an ion-selective electrode is responsible for the EMF response and selectivity of the entire electrode. Comment: Membranes of sensor electrodes are thought to be practically homogeneous, but an actual membrane may contain inhomogeneous regions, often at surfaces, and connected with materials and preparation methods used. Inhomogeneous regions include low dielectric polymer regions with few charge sites and regions with high local site densities. Surface regions of plasticized liquid membranes often are low in sites and high in plasticizer or exuded impurities.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2531

membrane potential

Synonymous with membrane emf.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 619

membrane sites

in an ion-selective electrode

Membranes frequently contain built-in 'fixed' charged sites (e.g. immobile $–(SO_3^-)$ in polystyrenesulfonate), or intentionally added, hydrophobically trapped, 'mobile' sites [e.g. tetraphenylborate in plasticized poly(vinyl chloride)]. Such membranes with charged sites are named sited membranes. Ions of opposite sign in the membrane are ' counter-ions '. Ions of the same sign as sites are not present in significant quantities, and are co-ions. Sited membranes are 'permselective' to counter-ions i.e. only counter-ions exchange into the membrane and therefore have some mobility in the membrane bulk.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2532

memory effect

in atmospheric chemistry

In instruments used for atmospheric trace component analysis, the dependence of an instrument reading on one or several previous sample(s).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2201

mer-

in inorganic nomenclature

An affix used in names to denote meridional; three groups occupying vertices of an octahedral coordination sphere in such a relationship that one is *cis* to the two others which are themselves *trans*, not now recommended for precise nomenclature purposes.

Source:
Red Book, p. 245

mercaptals [obsolete]

A term once used for dithioacetals derived from aldehydes; its use is discouraged.
See: thioacetals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

mercaptans [obsolete]

A traditional term abandoned by IUPAC, synonymous with thiols. This term is still widely used.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

mercaptides [obsolete]

An obsolescent synonym for thiolates.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

mercaptoles [obsolete]

An archaic term for dithioketals.
See: thioacetals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

mercury flow system

Also contains definitions of: open dynamic system *in spectrochemical analysis*, open static system *in spectrochemical analysis*

in spectrochemical analysis

For mercury released directly as atomic vapour, different direct transfer systems are used. In an open dynamic system the liberated analyte is transported by a carrier gas through the sampling or excitation source and swept away. In an open static system the equilibrated gaseous phase is forced into the absorption cell by displacement, e.g. by water. During measurement the gaseous phase is thus static. In a closed system the analyte and carrier gas are circulated through the absorption cell and the generator vessel until equilibrium between the liquid and gaseous phases is established.

Source:
PAC, 1992, *64*, 261 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XIII. Terms related to chemical vapour generation (IUPAC Recommendations 1992))* on page 263

mercury–xenon lamp

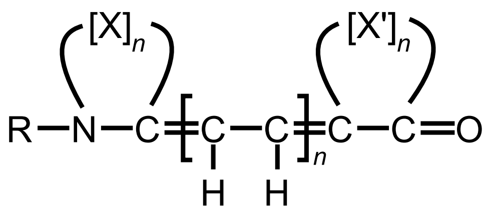
Synonym: mercury–xenon arc

Non-coherent intense source of ultraviolet, visible, and near-infrared radiation produced by an electrical discharge in a mixture of mercury vapour and xenon under high pressure.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 369

mero

A prefix meaning part, partial or fragment, used in formation of compound words, e.g. merocyanines are compounds related to cyanines but have a nitrogen atom at only one end of the chromogenic system instead of at both ends.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1348

merry-go-round reactor (turntable reactor)

An apparatus in which several samples are rotated around a radiation source in order to expose each to equal amounts of radiation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2254

meso

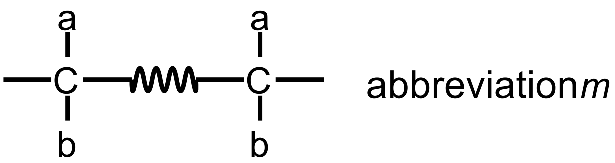
A prefix to indicate the presence of a symmetry element of the second kind (see chirality) in a chemical species which is usually one of a set of diastereoisomers that also includes a chiral member.
See: meso-compound

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2211

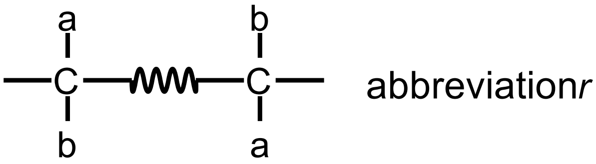
meso structures

in polymers

Relative configurations of consecutive, but not necessarily contiguous, constitutionally equivalent carbon atoms that have a symmetrically-constituted connecting group (if any) are designated 'meso' or 'racemo', as appropriate. Examples:



meso



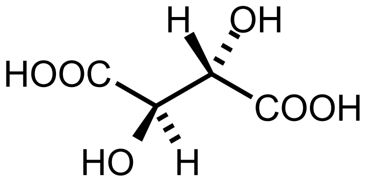
racemo

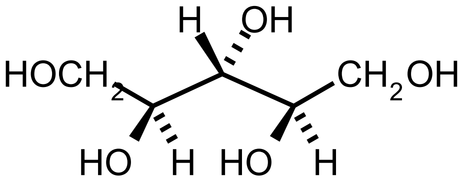
(The symbol  represents a symmetrically-constituted connecting group, such as –CH_2–, –CH_2–CH_2–, or –CR_2–CH_2–CR_2–.)

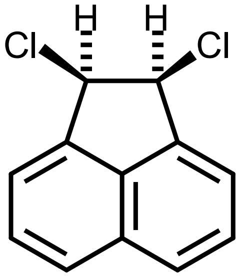
Source:
Purple Book, p. 37

meso-compound

A term for the achiral member(s) of a set of diastereoisomers which also includes one or more chiral members. For example:







Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2211

mesogen

A compound that under suitable conditions of temperature, pressure, and concentration can exist as a mesophase or, in particular, as a liquid-crystal (LC) phase.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 497

mesogenic group

A part of a molecule or macromolecule endowed with sufficient anisotropy in both attractive and repulsive forces to contribute strongly to mesophase or, in particular, liquid-crystal mesophase formation in low-molar-mass and polymeric substances.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 497

mesogenic monomer

A monomer which can impart the properties of liquid crystals to the polymers formed by its polymerization.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2304

mesogenic pitch

A pitch with a complex mixture of numerous essentially aromatic hydrocarbons. It does not contain anisotropic particles detectable by optical microscopy. Mesogenic pitch is low in quinoline-insoluble fractions and capable of transforming into mesophase pitch during continuous heat treatment above $750\ \mathrm{K}$ by the formation of optically detectable carbonaceous mesophase.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 496

mesoionic compounds

Dipolar five- (possibly six-) membered heterocyclic compounds in which both the negative and the positive charge are delocalized, for which a totally covalent structure cannot be written, and which cannot be represented satisfactorily by any one polar structure. The formal positive charge is associated with the ring atoms, and the formal negative charge is associated with ring atoms or an exocyclic nitrogen or chalcogen atom. Mesoionic compounds are a subclass of betaines.
See also: munchnones, sydnones

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1349

mesolytic cleavage

Cleavage of a bond in a radical ion whereby a radical and an ion are formed. The term reflects the mechanistic duality of the process, which can be viewed as homolytic or heterolytic depending on how the electrons are attributed to the fragments.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1139

mesomeric effect

Also contains definition of: resonance effect

The effect (on reaction rates, ionization equilibria, etc.) attributed to a substituent due to overlap of its p- or π-orbitals with the p- or π-orbitals of the rest of the molecular entity. Delocalization is thereby introduced or extended, and electronic charge may flow to or from the substituent. The effect is symbolized by M. Strictly understood, the mesomeric effect operates in the ground electronic state of the molecule. When the molecule undergoes electronic excitation or its energy is increased on the way to the transition state of a chemical reaction, the mesomeric effect may be enhanced by the electromeric effect, but this term is not much used, and the mesomeric and electromeric effects tend to be subsumed in the term resonance effect of a substituent.
See also: electronic effect, field effect, inductive effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1139

mesomerism

Essentially synonymous with resonance. The term is particularly associated with the picture of π-electrons as less localized in an actual molecule than in a Lewis formula. The term is intended to imply that the correct representation of a structure is intermediate between two or more Lewis formulae.
See also: aromatic (2), delocalization

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1139

mesomorphic phase

Also contains definition of: nematic state

Often formed by concentrated systems of surfactants. These are states of matter in which anisometric molecules (or particles) are regularly arranged in one (nematic state) or two (smectic state) directions, but randomly arranged in the remaining direction(s).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

mesomorphic state

A state of matter in which the degree of molecular order is intermediate between the perfect three-dimensional, long-range positional and orientational order found in solid crystals and the absence of long-range order found in isotropic liquids, gases, and amorphous solids.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 495

mesomorphic transition

A transition that occurs between a fully-ordered crystalline solid and an isotropic liquid. Mesomorphic transitions can occur (i) from a crystal to a liquid crystal (ii) from a liquid crystal to another liquid crystal and (iii) from a liquid crystal to an isotropic liquid.
See: liquid-crystal transitions

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 586

mesopause

in atmospheric chemistry

That region of the atmosphere between the mesosphere and the thermosphere at which the temperature is a minimum.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2201

mesophase

A phase occurring over a definite range of temperature, pressure, or concentration within the mesomorphic state.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 495

mesophase pitch

A pitch with a complex mixture of numerous essentially aromatic hydrocarbons containing anisotropic liquid-crystalline particles (carbonaceous mesophase) detectable by optical microscopy and capable of coalescence into the bulk mesophase.
Note:
The carbonaceous mesophase particles are formed from the aromatics of high molecular mass in mesogenic pitch, which have not yet been aggregated to particles detectable by optical microscopy within the apparently isotropic pitch matrix. The carbonaceous mesophase is insoluble in quinoline and pyridine, but the amount of mesophase measured from microscopical observation appears somewhat higher because parts of the carbonaceous mesophase can be extracted by the solvents.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 496

mesophase pitch-based carbon fibres

Synonym: MPP-based carbon fibres

Mesophase pitch-based carbon fibres (MPP-based carbon fibres) are carbon fibres obtained from mesogenic pitch after it has been transformed into mesophase pitch (MPP) at least during the process of spinning, and after the spun mesophase pitch fibres have been made non-fusible (stabilized) and carbonized.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 496

mesophiles

Microorganisms which grow at moderate temperatures in the range 20 – 45 °C, and which have an optimum growth temperature in the range 30 – 39 °C.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 160

mesopore
in catalysis

Pore of intermediate size. [Those with widths exceeding about 0.05 μm or 50 nm (500 Å) are called macropores; those with widths not exceeding about 2 nm (20 Å) are called micropores].

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 585
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

mesoscale

In meteorology, the size or scale of phenomena smaller than ordinary cyclones or weather systems but larger than such microscale phenomena as the thickness of the boundary layer, the wakes of objects, etc. Thunderstorms involve mesoscale processes, and other meteorological events the size of cities are usually mesoscale processes.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2201

mesosphere

That region of the atmosphere which lies above the stratopause (about 4752 km) and below the mesopause (about 8090 km) and in which temperature decreases with increasing height; this is the region in which the lowest temperatures of the atmosphere occur.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2201

messenger RNA (mRNA)

An RNA molecule that transfers the coding information for protein synthesis from the chromosomes to the ribosomes. mRNA is formed from a DNA template by transcription. It may be a copy of a single gene or of several adjacent genes (polycistronic mRNA). On the ribosome, the sequence is converted into the programmed amino acid sequence through translation.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 160

metabolic half-life (metabolic half-time)

Time required for one-half of the quantity of a substance in the body to be metabolised.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1059

metabolism

The entire physical and chemical processes involved in the maintenance and reproduction of life in which nutrients are broken down to generate energy and to give simpler molecules (catabolism) which by themselves may be used to form more complex molecules (anabolism). In case of heterotrophic organisms, the energy evolving from catabolic processes is made available for use by the organism.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 160

metabolite

Any intermediate or product resulting from metabolism.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 160

metal to ligand charge transfer (MLCT) transition

An electronic transition of a metal complex that corresponds to excitation populating an electronic state in which considerable electron transfer from the metal to a ligand has occurred.
See also: ligand to metal charge transfer transition

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2254

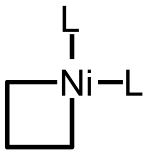
metal to metal charge transfer (MMCT) transition

An electronic transition of a bi- or poly-nuclear metal complex that corresponds to excitation populating an electronic state in which considerable electron transfer between two metal centres has occurred.
See also: intervalence charge transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2254

metallacycloalkanes

Monocyclic compounds containing a metal atom and saturated carbon atoms as ring members, e.g.:

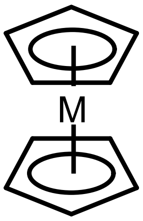


L is a ligand, e.g. triphenylphosphane

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1349

metallocenes

Organometallic coordination compounds in which one atom of a transition metal such as iron, ruthenium or osmium is bonded to and only to the face of two cyclopentadienyl [η^5-(C_5H_5)] ligands which lie in parallel planes. The term should not be used for analogues having rings other than cyclopentadienyl as ligands.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1349

metalloenzyme

An enzyme that, in the active state, contains one or more metal ions which are essential for its biological function.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1284

metallurgical coke

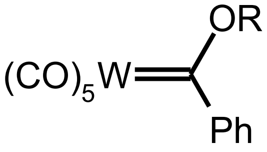
Metallurgical coke is produced by carbonization of coals or coal blends at temperatures up to 1400 K to produce a macroporous carbon material of high strength and relatively large lump size.
Note:
Metallurgical cokes must have a high strength to support heavy loads in the blast furnace without disintegration. Metallurgical coke is also used as filler coke for polygranular carbon products.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 497

metal–carbene complexes

Synonym: carbene metal complexes

Metal complexes of the type R_2CML_n (M = metal, L = ligand) in which formally a carbene is coordinated to a metal, e.g.

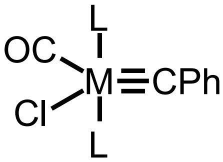


Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1349

metal–carbyne complexes

Synonym: carbyne metal complexes

Metal complexes of the type $RCML_n$ (M = metal, L = ligand) in which formally a carbyne is coordinated to a metal, e.g.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1349

metal–insulator transition

Synonym: metal–nonmetal transition

A transition characterized by a sudden change in electrical transport properties (conductivity) due to a reversible change from localized to itinerant behaviour of the electrons. Example: The transition at 339 K in VO_2 where it changes from a high-temperature metallic behaviour to a low-temperature semiconductor behaviour. Synonymous with metal–nonmetal transition.
See: localized-itinerant transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 586

metamagnetic transition

An antiferromagnetic to ferromagnetic transition for $H_{\mathrm{applied}} > H_{\mathrm{c}}$ and/or $T > T_{\mathrm{t}}$ where H_{c} and T_{t} refer to the critical magnetic field and transition temperature, respectively.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 586

metastability

of a phase

A term that describes the state of a phase in which an energy barrier considerably higher than $k\,T$ must be surmounted before this phase can transform to a phase of lower molar Gibbs energy and molar Helmholtz energy, where k is the Boltzmann constant and T the thermodynamic temperature.
Note:
In a thermodynamic sense, the equilibrium state is the state with the lowest molar Gibbs energy; a metastable state corresponds to a relative minimum in the molar Gibbs energy.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 586

metastable

See: metastable state *in nuclear chemistry*, metastable state *in spectrochemistry*, metastable ion *in mass spectrometry*, transient (chemical) species

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 609
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1463
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1139
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

metastable ion

in mass spectrometry

An ion which is formed with sufficient excitation to dissociate spontaneously during its flight from the ion source to the detector.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

metastable state

in nuclear chemistry

An isomeric state in an energy state higher than the ground state.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

metastable state

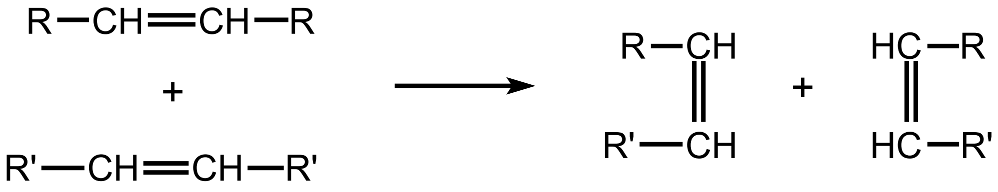
in spectrochemistry

Any excited state which in principle, by virtue of the selection rules, cannot radiatively combine with any lower state. It usually has a considerably longer lifetime than an ordinary excited state.

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1463

metathesis

A bimolecular process formally involving the exchange of a bond (or bonds) between similar interacting chemical species so that the bonding affiliations in the products are identical (or closely similar) to those in the reactants. For example:



(The term has its origin in inorganic chemistry with a different meaning, but this older usage is not applicable in physical organic chemistry.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1139

methanogens

Strictly anaerobic archaebacteria, able to use only a very limited substrate spectrum (e.g. molecular hydrogen, formate, methanol, methylamine, carbon monoxide or acetate) as electron donors for the reduction of carbon dioxide to methane.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 160

method of isotopic perturbation

NMR shift difference measurement of the isotope effect on a fast (degenerate) equilibrium between two species which are equivalent except for isotopic substitution. This can be used to distinguish a rapidly equilibrating mixture with time-averaged symmetry from a single structure with higher symmetry.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1132

methylene

See: carbene

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1139

methylidyne

See: carbyne

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1140

methylotrophic microorganisms

Organisms that use, as substrates for growth, C compounds containing carbon in a lower oxidation state than in carbon dioxide.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 160

metre

SI base unit for length (symbol: m). The metre is the length of path travelled by light in vacuum during a time interval of $\frac{1}{299\,792\,458}$ of a second.

Source:
Green Book, 2nd ed., p. 70
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 981

micellar catalysis

The acceleration of a chemical reaction in solution by the addition of a surfactant at a concentration higher than its critical micelle concentration so that the reaction can proceed in the environment of surfactant aggregates (micelles). (Rate enhancements may be due, for example, to higher concentration of the reactants in that environment, more favourable orientation and solvation of the species, or enhanced rate constants in the micellar pseudophase of the surfactant aggregate.) Micelle formation can also lead to a decreased reaction rate.
See also: catalyst

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1140

micellar mass

The term usually refers to a neutral micelle and therefore includes an equivalent amount of counter-ions with the surfactant ions.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

micellar solubilization

Synonym: solubilization

In a system formed by a solvent, an association colloid and at least one other component (the solubilizate), the incorporation of this other component into or on the micelles is called micellar solubilization, or, briefly, solubilization.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

micelle

Surfactants in solution are often association colloids, that is, they tend to form aggregates of colloidal dimensions, which exist in equilibrium with the molecules or ions from which they are formed. Such aggregates are termed micelles.
See also: inverted micelle

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1140

micelle charge

Usually understood to include the net charge of the surfactant ions and the counterions bound to the micelle.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

Michaelis constant, K_m

Substance concentration of substrate at which the rate of reaction is equal to one half of the limiting rate (maximum rate). Notes

1. Also called the Michaelis concentration
2. The Michaelis constant (Michaelis concentration) may be used only when Michaelis–Menten kinetics is obeyed.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 981

Michaelis–Menten kinetics

The dependence of an initial rate of reaction upon the concentration of a substrate S that is present in large excess over the concentration of an enzyme or other catalyst (or reagent) E with the appearance of saturation behaviour following the Michaelis-Menten equation:

$$v = \frac{V\,[\mathrm{S}]}{K_{\mathrm{m}} + [\mathrm{S}]},$$

where v is the observed initial rate, V is its limiting value at substrate saturation (i.e. $[\mathrm{S}] \gg K_{\mathrm{m}}$), and K_{m} the substrate concentration when $v = \frac{V}{2}$. The definition is experimental, i.e. it applies to any reaction that follows an equation of this general form. The symbols V_{max} or v_{max} are sometimes used for V. The parameters V and K_{m} (the 'Michaelis constant') of the equation can be evaluated from the slope and intercept of a linear plot of v^{-1} *vs.* $[\mathrm{S}]^{-1}$ (a 'Lineweaver–Burk plot') or from slope and intercept of a linear plot of v *vs.* $\frac{v}{[\mathrm{S}]}$ ('Eadie–Hofstee plot'). A Michaelis–Menten equation is also applicable to the condition where E is present in large excess, in which case the concentration $[\mathrm{E}]$ appears in the equation instead of $[\mathrm{S}]$. The term has sometimes been used to describe reactions that proceed according to the scheme:

$$\mathrm{E} + \mathrm{S} \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} \mathrm{ES} \xrightarrow{k_{\mathrm{cat}}} \mathrm{Products}$$

in which case $K_{\mathrm{m}} = \frac{k_{-1} + k_{\mathrm{cat}}}{k_1}$ (Briggs–Haldane conditions). It has more usually been applied only to the special case in which $k_{-1} \gg k_{\mathrm{cat}}$ and $K_{\mathrm{m}} = \frac{k_{-1}}{k_1} = K_s$; in this case K_{m} is a true dissociation constant (Michaelis–Menten conditions).
See also: rate-determining step

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1140
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 172

Michaelis–Menten mechanism

The Michaelis–Menten mechanism is the simplest mechanism that will explain Michaelis–Menten kinetics According to the mechanism, a substrate A first combines with a molecule of enzyme E, and this process is followed by a step in which the enzyme-substrate complex EA breaks down (sometimes with the participation of the solvent) into enzyme and reaction products:

$$\mathrm{E} + \mathrm{A} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{EA} \xrightarrow{k_2} \mathrm{E} + \mathrm{Products}$$

If, as is usual, the substrate A is present in great excess of the enzyme it can be shown that steady-state conditions apply, and that the rate equation is:

$$v = \frac{k_2\,[\,\mathrm{E}\,]_0\,[\,\mathrm{A}\,]}{\frac{k_{-1}+k_2}{k_1} + [\,\mathrm{A}\,]}$$

where $[\,\mathrm{E}\,]_0$ is the total concentration of enzyme. This equation is of the form of the Michaelis–Menten equation. Other, more complicated, mechanisms lead to the Michaelis–Menten equation, adherence to which therefore does not require that the Michaelis– Menten mechanism applies.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 172

micro

SI prefix for 10^{-6} (symbol: μ).

Source:
Green Book, 2nd ed., p. 74

micro-network

Polymer network that has dimensions of the order of $1\ \mathrm{nm}$ to $1\ \mu\mathrm{m}$.
Note:
Modified from previous version. The definition proposed here is recommended as being more explicit.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1814

microbial leaching

A process for the solubilization of metals, mostly from poor ores, by lithotrophic bacteria.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 158

microcanonical rate constant

A rate constant calculated by microcanonical variational transition-state theory and therefore a rate constant that relates to a fixed energy.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 173

microcanonical variational transition-state theory (μVTST)

A development of transition-state theory in which the dividing surface is varied so as to minimize the rate calculated for a fixed energy. The rate expressions obtained in a microcanonical treatment can be integrated over the energy, taking into account the statistical distribution over energy states, so as to give the canonical, or thermal, rates.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 173

microcarrier

in biotechnology

A small, beaded material, derived from silica, glass, dextran or similar materials, used for the immobilization of biocatalysts or as a support for the culture of anchorage-dependent animal cell lines.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 160

microclimatology

The science that deals with the climate of restricted areas and investigates their phenomena and causes.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2201

microdomain morphology

Morphology consisting of phase microdomains.
Notes:

1. Microdomain morphologies are usually observed in block, graft, and segmented copolymers.
2. The type of morphology observed depends upon the relative abundance of the different types of structural units and the conditions for the generation of the morphology. The most commonly observed morphologies are spheres, cylinders, and lamellae.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2004

microelectrophoresis

The electrophoresis technique involving the movement of a mass of particles on a small scale (e.g. paper electrophoresis).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

microfiltration

Pressure-driven membrane-based separation process in which particles and dissolved macromolecules larger than $0.1\ \mu m$ are rejected.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1487

microgel

Also contains definition of: gel microparticle

Particle of gel of any shape with an equivalent diameter of approximately 0.1 to $100\ \mu m$.
Note:
The definition proposed here is recommended for its precision and because it distinguishes between a microgel and a nanogel.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1807

microheterogeneity

in biochemistry

A particular glycoprotein may occur in forms that differ in the structure of one or more or its carbohydrate units, a phenomenon known as microheterogeneity.

Source:
PAC, 1988, *60*, 1389 *(Nomenclature of glycoproteins, glycopeptides and peptidoglycans (Recommendations 1985))* on page 1391
White Book, p. 86

micrometeorology

The study of the meteorological processes on scales from a millimeter or less up to tens or hundreds of metres; e.g. meteorology of a local site that is usually small and often is confined to a shallow layer of air next to the ground.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202

microphotometer

The optical instrument used to measure transmittance in atomic emission spectroscopy.

Source:
Orange Book, p. 160

micropore filling

in catalysis

The process in which molecules are adsorbed in the adsorption space within micropores.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 588
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

micropore

in catalysis

Pore with width not exceeding about $2.0\ \mathrm{nm}$ $(20\ \mathrm{\AA})$.
Cf. macropore *in catalysis*, mesopore *in catalysis*
.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 585
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

micropore volume

in catalysis

Conventionally measured by the volume of the adsorbed material which completely fills the micropores expressed in terms of bulk liquid at atmospheric pressure and at the temperature of measurement.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 588
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

microporous carbon

A porous carbon material, usually a char or carbon fibres, which may or may not have been subjected to an activation process to increase its adsorptive properties. A microporous carbon is considered to have a major part of its porosity in pores of less than $2\ \mathrm{nm}$ width and to exhibit apparent surface areas usually higher than 200 to $300\ \mathrm{m^2\ g^{-1}}$.
Note:
The surface areas determined by the Brunauer–Emmett–Teller (BET) method are apparent surface areas only since the BET adsorption equation is, in principle, not valid when micropore filling occurs. The determination of the true surface area in the micropores depends on the method used for the evaluation of the adsorption isotherms and on the model used for the shape of the micropores (cylindrical, slit-shaped or other).
See: micropore

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 497

See also:
PAC, 1972, *31*, 503 *(Méthodes nouvelles d'accès électrochimique et de calcule numérique relatives aux constantes de stabilité des polycomplexes)* on page 518

microscopic chemical event

See: chemical reaction, molecularity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1140

microscopic cross-section, σ

A measure of the probability of a specified interaction or reaction between an incident radiation and a target particle or system of particles. It is the reaction rate per target particle for a specified process divided by the flux of the incident radiation. In general, a specification is added of the type of radiation (e.g. neutron, photon), the energy of the incident radiation (e.g. thermal, epithermal, fast) and the type of interaction of reaction (e.g. activation, fission, scattering).
See also: macroscopic cross-section

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517
Orange Book, p. 217

microscopic diffusion control (encounter control)

The observable consequence of the limitation that the rate of a bimolecular chemical reaction in a homogeneous medium cannot exceed the rate of encounter of the reacting molecular entities. If

(hypothetically) a bimolecular reaction in a homogeneous medium occurred instantaneously when two reactant molecular entities made an encounter, the rate of reaction would be an encounter-controlled rate, determined solely by rates of diffusion of reactants. Such a hypothetical 'fully diffusion controlled rate' is also said to correspond to 'total microscopic diffusion control', and represents the asymptotic limit of the rate of reaction as the rate constant for the chemical conversion of the encounter pair into product (or products) becomes large relative to the rate constant for separation (or dissociation) of the encounter pair. 'Partial microscopic diffusion control' is said to operate in a homogeneous reaction when the rates of chemical conversion and of separation are comparable. (The degree of microscopic diffusion control cannot usually be determined with any precision.)
See also: mixing control

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1140

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 173

microscopic electrophoresis

A technique in which the electrophoresis of individual particles is observed with the aid of a microscope or ultra-microscope.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

microscopic film

A film which has lateral dimensions in the range $0.1 - 100\ \mu\text{m}$.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1671

microscopic kinetics

This term applies to a kinetic study in which the emphasis is on the interpretation of the behaviour in terms of elementary reactions.
See: macroscopic kinetics, molecular kinetics

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 173

microscopic reversibility at equilibrium

The principle of microscopic reversibility at equilibrium states that, in a system at equilibrium, any molecular process and the reverse of that process occur, on the average, at the same rate. This definition corresponds to the statement of the principle that was given by R.C. Tolman in 1924. However, many workers have interchanged the meanings of microscopic reversibility and detailed balance, and it seems best now to regard the two, which are closely related, as synonymous.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 173

microsome

Artefactual spherical particle, not present in the living cell, derived from pieces of the endoplasmic reticulum present in homogenates of tissues or cells: microsomes sediment from such homogenates when centrifuged at 10^6 g and higher: the microsomal fraction obtained in this way is often used as a source of mono-oxygenase enzymes.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2070

microsyneresis

Syneresis in which the exudation of the liquid is from microscopic regions within a network.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1826

middle atmosphere

The combined stratosphere and mesosphere in the atmosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202

Mie scattering

The scattering of electromagnetic radiation by spherical particles of any size r, relative to the wavelength, λ. Since the cases $r \ll \lambda$ and $r \gg \lambda$ are covered by Rayleigh (dipole) scattering and geometric scattering theories, respectively, Mie scattering often refers to the case of $r \approx \lambda$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202

migration

Also contains definition of: bond migration

1. The (usually intramolecular) transfer of an atom or group during the course of a molecular rearrangement.
2. The movement of a bond to a new position, within the same molecular entity is known as 'bond migration'. Allylic rearrangements, e.g.

$$R{-}CH{=}CH{-}CH_2{-}X \longrightarrow R{-}\underset{\displaystyle X}{\underset{|}{C}}H{-}CH{=}CH_2$$

exemplify both types of migration.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1141

migration current

The difference between the current that is actually obtained, at any particular value of the potential of the indicator or working electrode, for the reduction or oxidation of an ionic electroactive substance and the current that would be obtained, at the same potential, if there were no transport of that substance due to the electric field between the electrodes. The sign convention regarding current is such that the migration current is negative for the reduction of a cation or for the oxidation of an anion, and positive for the oxidation of a cation or the reduction of an anion. Hence the migration current may tend to either increase or decrease the total current observed. In any event the migration current approaches zero as the transport number of the electroactive substance is decreased by increasing the concentration of the supporting electrolyte, and hence the conductivity

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1497

migration time, t_m

in capillary electrophoresis

The time required for the analyte to move through the effective length of the capillary, L_{eff}, that is, from the sample introduction point to the detection point.

Source:
PAC, 2004, *76*, 443 *(Terminology for analytical capillary electromigration techniques (IUPAC Recommendations 2003))* on page 448

migration time of micelles, t_{mc}

in micellar electrokinetic chromatography

Experimentally determined as the migration time of a compound that is completely retained in the micellar phase.

Source:
PAC, 2004, *76*, 443 *(Terminology for analytical capillary electromigration techniques (IUPAC Recommendations 2003))* on page 449

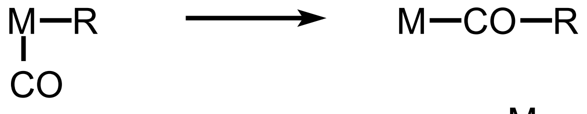
migratory aptitude

The term is applied to characterize the relative tendency of a group to participate in a rearrangement. In nucleophilic rearrangements (migration to an electron-deficient centre), the migratory aptitude of a group is loosely related to its capacity to stabilize a partial positive charge, but exceptions are known, and the position of hydrogen in the series is often unpredictable.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1141

migratory insertion

A combination of migration and insertion. The term is mainly used in organometallic chemistry.



$$\underset{\mathrm{CO}}{\mathrm{M}}\mathrm{-R} \longrightarrow \mathrm{M-CO-R}$$

M = metal

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1141

milli

SI prefix for 10^{-3} (symbol: m).

Source:
Green Book, 2nd ed., p. 74

milligram equivalent of readability

of a precision balance

The product of readability and the value of the scale division (in mg per division).

Source:
Orange Book, p. 36

millimetre of mercury

Non-SI unit for pressure; $\mathrm{mmHg} \approx 133.322\ \mathrm{Pa}$. This old unit is not recognized by CIPM or ISO, but it is used for blood pressure.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 981

milling (grinding)

The mechanical reduction of the particle size of a sample by attribution (friction), impact or cutting. The required particle size of a sample is related to the size of the test portion and the number of particles required to ensure homogeneity among test portions. The reduction in particle size may sometimes result in particles of different hardness and density, which produces inhomogeneity during the preparation of the test sample or during the withdrawal of the test portion.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1205

minimum consumption time, t_{min}

in flame emission and absorption spectrometry

The time during which nebulization must be carried out in order to perform one analysis with a given precision. The minimum consumption time is equal to the minimum volume consumed of the prepared sample divided by the rate of fluid consumption in order to obtain a given precision. It can be reduced by means of integrating the signal or measuring the signal increments (kinetic methods).

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1740

minimum density of states criterion

This is a criterion used in Rice–Ramsperger–Kassel–Marcus (RRKM) theory for locating the transition state. The reaction coordinate r at the transition state, according to this criterion, is given by $\frac{\partial(N(\varepsilon_{\mathrm{r}}))}{\partial r} = 0$, where $N(\varepsilon_{\mathrm{r}})$ is the density of states at an internal energy ε_{r}.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 174

minimum lethal concentration (LC_{min})

Synonym: lowest lethal concentration found

Lowest concentration of a toxic substance in an environmental medium that kills individual organisms or test species under a defined set of conditions. Synonymous with lowest lethal concentration found.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2071

minimum lethal dose (LD_{min})

Lowest amount of a substance that, when introduced into the body, may cause death to individual species of test animals under a defined set of conditions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2071

minimum-energy reaction path

Acronym: MERP

Path orthogonal to the equipotential contours of a potential energy surface that connects the energy minima through a saddle point (transition state) from which it slopes downwards along the steepest descending lines in $3N - 6$ configurational space (N is the number of nuclei in the reacting system).
Note:
MERP calculation allows the investigation of detailed changes in molecular structure describing the transformation of reactants to products.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 370

minute

of arc

Non-SI unit of plane angle.

$$1' = (1/60)\,^\circ = 2.908\,882\,... \times 10^{-4}\,\mathrm{rad}.$$

Source:
Green Book, 2nd ed., p. 113
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 981

miscibility

Capability of a mixture to form a single phase over certain ranges of temperature, pressure, and composition.
Notes:

1. Whether or not a single phase exists depends on the chemical structure, molar-mass distribution, and molecular architecture of the components present.
2. The single phase in a mixture may be confirmed by light scattering, X-ray scattering, and neutron scattering.
3. For a two-component mixture, a necessary and sufficient condition for stable or metastable equilibrium of a homogeneous single phase is

   $$\left(\frac{\partial^2 \Delta_{\mathrm{mix}} G}{\partial \phi^2}\right)_{T,p} > 0,$$

   where $\Delta_{\mathrm{mix}} G$ is the Gibbs energy of mixing and ϕ the composition, where ϕ is usually taken as the volume fraction of one of the components. The system is unstable if the above second derivative is negative. The borderline (spinodal) between metastable and unstable states is defined by the above second derivative equalling zero. If the compositions of two conjugate (coexisting) phases become identical upon a change of temperature or pressure, the third derivative also equals zero (defining a critical state).
4. If a mixture is thermodynamically metastable, it will demix if suitably nucleated. If a mixture is thermodynamically unstable, it will demix by spinodal decomposition or by nucleation and growth if suitably nucleated, provided there is minimal kinetic hindrance.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1987

miscibility gap

Area within the coexistence curve of an isobaric phase diagram (temperature *vs* composition) or an isothermal phase diagram (pressure *vs* composition).
Note:
A miscibility gap is observed at temperatures below an upper critical solution temperature (UCST) or above the lower critical solution temperature (LCST). Its location depends on pressure. In the miscibility gap, there are at least two phases coexisting.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1996

mist

in atmospheric chemistry

A qualitative term applied to a suspension of droplets in a gas. In the atmosphere a mist produces a generally thin, greyish veil over the landscape. It reduces visibility to a lesser extent than fog but somewhat more than haze (visibility of less than $2\ \mathrm{km}$ but greater than $1\ \mathrm{km}$).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202

mitochondria

Organelles appearing in all eukaryotic cells which produce ATP as useful energy for the cell by oxidative phosphorylation. The proteins for the adenosine 5'-triphosphate (ATP)-generating electron transport of the respiration chain are located in the inner mitochondrial membrane. Mitochondria contain many enzymes of the citric acid cycle and for fatty acid β-oxidation. Many of them are coded for by nuclear DNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 160
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2071

mitosis

The process whereby a cell nucleus divides into two daughter nuclei, each having the same genetic complement as the parent cell.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 161

mixed ceramic

Ceramic material consisting of co-continuous interpenetrating networks of two or more metal carbides, nitrides or oxides.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1812

mixed control

See: transport control

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1838

mixed crystal (solid solution)

A crystal containing a second constituent which fits into and is distributed in the lattice of the host crystal. (The use of 'solid solution' for amorphous materials is not recommended.)

Source:
Orange Book, p. 85

mixed energy release

This is an effect found in a process A + BC when the attacking species A is heavy. Because A is heavy the A–B distance continues to decrease while the repulsive energy of B–C is being released.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 174

mixed indicator

An indicator containing a supplementary dye selected to heighten the overall colour change.

Source:
Orange Book, p. 48

mixed labelled

A specifically labelled compound is referred to as mixed labelled when the isotopically substituted compound has more than one kind of modified atom e.g. $CH_3–CH_2–[^{18}O][^2H]$.

Source:
Blue Book, p. 515
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1893

mixed potential

The value of the potential of a given electrode with respect to a suitable reference electrode when appreciable contributions to the total anodic and/or cathodic partial currents are made by species belonging to two or more different couples, but the total current is zero, i.e.

$$I = \sum_i I_i = 0 \quad (I_i \neq 0)$$

where I_i is the partial current of reaction i

$$I_i = I_{i,a} + I_{i,c}$$

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 513

mixing control

The experimental limitation of the rate of reaction in solution by the rate of mixing of solutions of the two reactants. It can occur even when the reaction rate constant is several powers of 10 less than that for an encounter-controlled rate. Analogous (and even more important) effects of the limitation of reaction rates by the speed of mixing are encountered in heterogeneous (solid/liquid, solid/gas, liquid/gas) systems.
See also: microscopic diffusion control, stopped flow

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1141
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 174

mixing height

in atmospheric chemistry

The height to which significant mixing of added pollutants occurs within the atmosphere. In reference to stack gases, it is considered the height at which stack effluent begins mixing with the atmosphere as it leaves the stack.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202

mixing

in analytical chemistry

The combining of components, particles or layers into a more homogeneous state. The mixing may be achieved manually or mechanically by shifting the material with stirrers or pumps or by revolving or shaking the container. The process must not permit segregation of particles of different size or properties. Homogeneity may be considered to have been achieved in a practical sense when the sampling error of the processed portion is negligible compared to the total error of the measurement system.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1204

mixing ratio

in atmospheric chemistry

In meteorology, the dimensionless ratio of the mass of a substance (such as water vapour) in an air parcel to the mass of the remaining substances in the air parcel. For trace substances, this is approximated by the ratio of the mass of the substance to the mass of air. However, in the case of water vapour the mass of dry air is used. In atmospheric chemistry, mixing ratios (molecular, molar, by volume, as well as by weight) are used to describe relative concentrations of atmospheric trace gases and impurities.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202

mixture

Portion of matter consisting of two or more chemical substances called constituents.

Source:
Physical Chemistry Division, unpublished

See also:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 535

MLCT

Abbreviation for Metal to Ligand Charge Transfer.

Source:
PAC, 1988, *60*, 1055 *(Glossary of terms used in photochemistry (Recommendations 1988))* on page 1078

mobile adsorption

Also contains definition of: non-localized adsorption

A situation in which molecules of adsorbate are free to move about the surface. Mobility of the adsorbate will increase with temperature and mobile adsorption may be either localized or non-localized. In localized mobile adsorption the adsorbate spends most of the time on the adsorption sites but can migrate or be desorbed and readsorbed elsewhere. In non-localized adsorption the mobility is so great that a small fraction of the adsorbed species is on the desorption sites and a large fraction at other positions on the surface.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

mobile phase

in chromatography

A fluid which percolates through or along the stationary bed, in a definite direction. It may be a liquid (liquid chromatography) or a gas (gas chromatography) or a supercritical fluid (supercritical-fluid chromatography). In gas chromatography the expression carrier gas may be used for the mobile phase. In elution chromatography the expression 'eluent' is also used for the mobile phase.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 824
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202
Orange Book, p. 97

mobile-phase velocity, u

in chromatography

The linear velocity of the mobile phase across the average cross-section of the chromatographic bed or column.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 840

mobility, μ

Drift velocity of electrons or holes divided by the electric field strength.
See also: electric mobility

Source:
Green Book, 2nd ed., p. 37

mobility (general)

Mass transport is described by a mobility b, defined by:

$$b_i = \frac{\nu_i}{\boldsymbol{F}_i}$$

where ν_i is the average drift velocity and $\boldsymbol{F}_i$ is the force on particle i.

Source:
PAC, 1999, *71*, 1307 *(Definitions of Terms for Diffusion in the Solid State)* on page 1319

mobility

in aerosol physics

The velocity of a particle per unit applied force.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202

Möbius aromaticity

A monocyclic array of orbitals in which there is a single out-of-phase overlap (or, more generally, an odd number of out-of-phase overlaps) reveals the opposite pattern of aromatic character to Hückel systems; with $4\,n$ electrons it is stabilized (aromatic), whereas with $4\,n+2$ it is destabilized (antiaromatic). In the excited state $4\,n+2$ Möbius π-electron systems are stabilized, and $4\,n$ systems are destabilized. No examples of ground-state Möbius π-electron systems are known, but the concept has been applied to transition states of pericyclic reactions [***See:*** aromatic]. The name is derived from the topological analogy of such an arrangement of orbitals to a Möbius strip.
See also: Hückel $4\,n+2$ rule

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1141

mode

The value of the variable occurring with the greatest frequency in the series of observations. A bimodal distribution is one which contains two maxima. The use of mode when reporting results of chemical analysis is generally not recommended.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 603
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202

mode-locked laser

A laser in which many resonant modes are coupled in phase, to yield a train of very short pulses (e.g. ps pulses). The coupling of the modes is obtained by modulation of the gain in the resonator, and can be active (electro-optic modulation of the losses or of the pump intensity), or passive (with a saturable absorber).
See also: free-running laser

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2254

model network

Polymer network synthesized using a reactant or reactants of known molar mass or masses and chemical structure.
Notes:

1. A model network can be prepared using a non-linear polymerization or by crosslinking of existing polymer chains.
2. A model network is not necessarily a perfect network. If a non-linear polymerization is used to prepare the network, non-stoichiometric amounts of reactants or incomplete reaction can lead to

network containing loose ends. If the crosslinking of existing polymer chains is used to prepare the network, then two loose ends per existing polymer chain result. In the absence of chain entanglements, loose ends can never be elastically active network chains.
3. In addition to loose ends, model networks usually contain ring structures as network imperfections.
4. Loose ends and ring structures reduce the concentration of elastically active network chains and result in the shear modulus and Young´ s modulus of the rubbery networks being less than the values expected for a perfect network structure.
5. Physical entanglements between network chains can lead to an increase in the concentration of elastically active network chains and, hence, increases in the shear modulus and the Young´ s modulus above the values expected for a perfect network structure.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1814

moderation

in nuclear chemistry

Reduction of the neutron energy by scattering without appreciable capture.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

moderator

A material used to reduce the neutron energy by scattering without appreciable capture.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

modified active solid

in chromatography

An active solid the sorptive properties of which have been changed by some treatment.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 830
Orange Book, p. 98

modified Arrhenius equation

This is an extension of the simple Arrhenius equation in which the pre-exponential factor is proportional to T^n where T is the temperature and n a constant:

$$k = B\,T^n \exp(-E_a/RT)$$

B is a temperature-independent constant.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 174

modified sample

A sample or a known fraction of the parent population in which the analyte has been isolated or (usually) concentrated before being submitted to the laboratory. If the isolation or concentration occurs in the laboratory, the procedure is usually considered part of the preparation of the test sample from the laboratory sample (in-laboratory processing).

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1204

modifier

in solvent extraction

A substance added to a solvent to improve its properties e.g. by increasing the solubility of an extractant, changing interfacial parameters or reducing adsorption losses. Additives used to enhance extraction rates should be called accelerators or catalysts.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2381

modulus of elasticity, E

Synonym: Young's modulus

The normal stress divided by linear strain.

Source:
Green Book, 2nd ed., p. 12

Mohr amplification process

in analysis

The process in which iodide is oxidized to iodate to achieve a more favourable measurement.

Source:
PAC, 1982, *54*, 2553 *(Recommendations on use of the term amplification reactions)* on page 2555

moiety

In physical organic chemistry moiety is generally used to signify part of a molecule, e.g. in an ester R^1COOR^2 the alcohol moiety is R^2O. The term should not be used for a small fragment of a molecule.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1141

MOL file format

The MOL file format is used to encode chemical structures, substructures and conformations as text-based connection tables. It is used by MDL Information Systems Inc. (*e.g.*, in their MACCS or ISIS programs).

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1146

See also:
molfile
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1147

molal

See: molality

Source:
Green Book, 2nd ed., p. 42
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 982

molality, m, b

Amount of entities of a solute divided by the mass of the solvent

Source:
Green Book, 2nd ed., p. 42
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 982

molar

Adjective before the name of an extensive quantity generally meaning division by amount of substance to make it intensive. Molar volume is volume divided by amount of substance. In a few special cases molar is used to denote division by amount concentration (e.g. molar absorption coefficient).

Source:
Green Book, 2nd ed., p. 7
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 982

molar absorption coefficient, ε

Also contains definition of: molar decadic absorption coefficient

Absorbance divided by the absorption pathlength, l, and the amount concentration, c:

$$\varepsilon(\lambda) = \frac{1}{c\,l} \lg\left(\frac{P_\lambda^0}{P_\lambda}\right) = \frac{A(\lambda)}{c\,l}$$

where P_λ^0 and P_λ are, respectively, the incident and transmitted spectral radiant power.

Notes:

1. The term molar absorptivity for molar absorption coefficient should be avoided.
2. In common usage for l/cm and $c/\mathrm{mol\,dm^{-3}}$ (M), $\varepsilon(\lambda)$ results in $\mathrm{dm^3\,mol^{-1}\,cm^{-1}}$ ($\mathrm{M^{-1}\,cm^{-1}}$, the most commonly used unit), which equals $0.1\ \mathrm{m^2\,mol^{-1}}$ (coherent SI units).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 371

molar absorptivity

See: absorption coefficent

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 982

molar activity

in radiochemistry

For a specified isotope, the activity of the compound divided by the amount of the material in moles: $A_\mathrm{m} = \frac{A}{n}$.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515

molar conductivity

See: conductivity

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 512

molar refraction, *R*

Function of the refractive index, n, given by $R = V_m \frac{n^2 - 1}{n^2 + 2}$, where V_m is the molar volume.

Source:
Green Book, 2nd ed., p. 33

molar-mass exclusion limit

in polymers

The maximum value of the molar mass or molecular weight of molecules or particles, in a specific polymer solvent system, that can enter into the pores of the porous non-adsorbing material used in size-exclusion chromatography. For particles with molar mass or molecular weight larger than the exclusion limit the separation effect of the size-exclusion chromatography vanishes.

Source:
Purple Book, p. 69

molarity

Term sometimes used for amount concentration.

Source:
Green Book, 2nd ed., p. 42

mole

SI base unit for the amount of substance (symbol: mol). The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon-12. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.

Source:
Green Book, 2nd ed., p. 70
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 983

molecular anion

See: molecular ion

Source:
Orange Book, p. 205

PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

molecular beams

Also contains definitions of: beam-gas experiments, crossed molecular beams

A molecular beam is produced by allowing a gas at higher pressure to expand through a small orifice into a container at lower pressure. The result is a beam of particles (atoms, free radicals, molecules or ions) moving at approximately equal velocities, with few collisions occurring between them. In a crossed molecular-beam experiment a reaction is studied using collimated beams of reactant molecules. For a bimolecular reaction, beams of the two reactants are caused to impinge on one another, often at an angle of 90°. In a beam-gas scattering experiment a collimated beam is introduced into a gas, and the scattering patterns are observed.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 175

molecular cation

See: molecular ion

Source:
Orange Book, p. 205
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

molecular conformation

of a polymer

The conformation of the macromolecule as a whole. In the polymer literature, molecular conformation is sometimes referred to as macroconformation. In molecular conformations involving parallel stems, the latter may be confined to the same crystal or may also extend over several crystals.

Source:
Purple Book, p. 77

molecular connectivity index

A molecular connectivity index is a numeric descriptor derived from molecular topology.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1146

molecular design

Molecular design is the application of all techniques leading to the discovery of new chemical entities with specific properties required for the intended application.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1146

molecular dynamics

Synonymous with reaction dynamics.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 175

molecular dynamics
in drug design

Molecular dynamics is a simulation procedure consisting of the computation of the motion of atoms in a molecule or of individual atoms or molecules in solids, liquids and gases, according to Newton's laws of motion. The forces acting on the atoms, required to simulate their motions, are generally calculated using molecular mechanics force fields.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1146

molecular entity

Any constitutionally or isotopically distinct atom, molecule, ion, ion pair, radical, radical ion, complex, conformer etc., identifiable as a separately distinguishable entity. Molecular entity is used in this Compendium as a general term for singular entities, irrespective of their nature, while chemical species stands for sets or ensembles of molecular entities. Note that the name of a compound may refer to the respective molecular entity or to the chemical species, e.g. methane, may mean a single molecule of CH_4 (molecular entity) or a molar amount, specified or not (chemical species), participating in a reaction. The degree of precision necessary to describe a molecular entity depends on the context. For example 'hydrogen molecule' is an adequate definition of a certain molecular entity for some purposes, whereas for others it is necessary to distinguish the electronic state and/or vibrational state and/or nuclear spin, etc. of the hydrogen molecule.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1142

molecular formula

For compounds consisting of discrete molecules, a formula according with the relative molecular mass (or the structure).

Source:
Red Book, p. 45

molecular graph

The graph with differently labelled (coloured) vertices (chromatic graph) which represent different kinds of atoms and differently labelled (coloured) edges related to different types of bonds. Within the topological electron distribution theory, a complete network of the bond paths for a given nuclear configuration.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1951

molecular graph theory

The theory which deals with analyses of all consequences of connectivities inherent in molecular structure and chemical transformations. The theory does not produce numerical data but uses available data and searches for regularities that can be attributed to combinatorial and topological origins.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1951

molecular graphics

Molecular graphics is a technique for the visualization and manipulation of molecules on a graphical display device.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1146

molecular ion

in mass spectrometry

An ion formed by the removal from (positive ions) or addition to (negative ions) a molecule of one or more electrons without fragmentation of the molecular structure. The mass of this ion corresponds to the sum of the masses of the most abundant naturally occuring isotopes of the various atoms that make up the molecule (with a correction for the masses of the electron(s) lost or gained). For example, the mass of the molecular ion of ethyl bromide $C_2H_5{}^{79}Br$ will be 2×12 plus 5×1.0078246 plus 78.91839 minus the mass of the electron (m_e). This is equal to $107.95751\ \mathrm{u} - m_e$, u being the unified atomic mass unit based on the standard that the mass of the isotope $^{12}C = 12\ \mathrm{u}$ exactly.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549
Orange Book, p. 205

molecular kinetics

This term is applied to a kinetic study in which there is emphasis on the behaviour of the system at the molecular level.
See: macroscopic kinetics

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 175

molecular laser

A gas laser which makes use of electronic, vibrational or rotational energy levels in molecules. The molecules can be excited by an electric discharge, as in the case of the N_2 or CO_2 laser, by chemical reactions, as in the HF or DF lasers, or by another laser, as in the CH_3F far IR laser.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1920

molecular mechanics calculation

Synonym: force-field calculation

An empirical calculational method intended to give estimates of structures and energies for conformations of molecules. The method is based on the assumption of 'natural' bond lengths and angles, deviation from which leads to strain, and the existence of torsional interactions and attractive and/or repulsive van der Waals and dipolar forces between non-bonded atoms. The method is also called '(empirical) force-field calculations'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1142

molecular metal

A non-metallic material whose properties resemble those of metals, usually following oxidative doping; e.g. polyacetylene following oxidative doping with iodine.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1142

molecular modeling

Molecular modeling is the investigation of molecular structures and properties using computational chemistry and graphical visualization techniques in order to provide a plausible three-dimensional representation under a given set of circumstances.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1147

molecular nucleation

in polymers

The initial crystallization of a small portion of a macromolecule, after which further crystallization is thermodynamically favoured. Molecular nucleation may give rise to a new crystal or increase the size of a pre-existing one.

Source:
Purple Book, p. 85

molecular orbital

A one-electron wavefunction describing an electron moving in the effective field provided by the nuclei and all other electrons of a molecular entity of more than one atom. Such molecular orbitals can be transformed in prescribed ways into component functions to give 'localized molecular orbitals'. Molecular orbitals can also be described, in terms of the number of nuclei (or 'centres') encompassed, as two-centre, multi-centre, etc. molecular orbitals, and are often expressed as a linear combination of atomic orbitals. An orbital is usually depicted by sketching contours on which the wavefunction has a constant value (contour map) or by indicating schematically the envelope of the region of space in which there is an arbitrarily fixed high (say 96%) probability of finding the electron occupying the orbital, giving also the algebraic sign (+ or −) of the wavefunction in each part of that region.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1142
Green Book, 2nd ed., p. 18

molecular orientation

Absorption probability (referred to electric dipolar absorption) for a molecular transition with its electric transition (dipole) moment at an angle θ with the electric vector of the light is proportional to $\cos^2\theta$. For the whole sample it is proportional to the orientation factor $K_\theta = \ <\cos^2\theta>$, averaged over all sample molecules. This average is 1 for a sample with all transition moments perfectly aligned along the electric vector of the light, $1/3$ for an isotropic sample and 0 for a sample where all transition moments are perpendicular to the electric vector.
Notes:

1. The directional cosines provide, especially for uniaxial samples, a simple description of exactly those orientation properties of the sample that are relevant for light absorption. With the principal coordinate system (x, y, z), forming angles $\theta = \alpha$, β, γ with the light electric vector in the z direction, all orientation effects induced by light absorption are contained in $K_{\theta\theta} = K_{\theta}$. Since the sum of K_{θ} for three perpendicular molecular axes is equal to 1, only two independent parameters are required to describe the orientation effects on light absorption.
2. A related, commonly used description is based on diagonalized Saupe matrices:

   $$S_{\theta} = (3K_{\theta} - 1)/2$$

   The principal (molecular) coordinate system (x, y, z) forming angles $\theta = \alpha$, β, γ with the light electric vector should be chosen such that the matrix K and the tensor S_{θ} are diagonal.

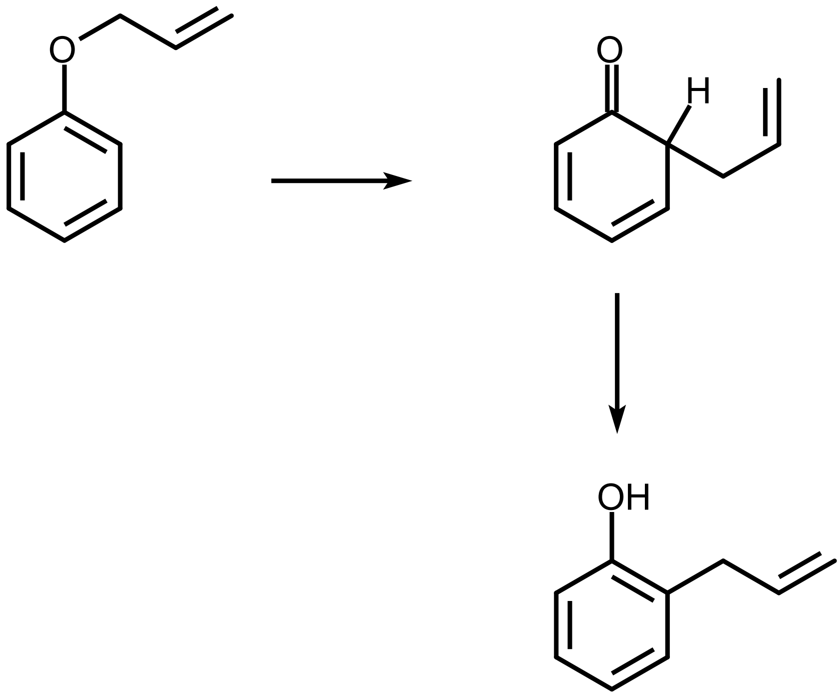
   To describe processes involving two or more photons, such as luminescence of a uniaxial, aligned sample, an expansion of the directional cosines to the fourth power is required.
3. Order parameters (related to Wigner matrices) are an alternative to the directional cosine-based description of molecular alignment. Order-parameter methods also work well for non-uniaxial samples and provide a seemingly more complex, but in other ways convenient, description of molecular orientation distributions. Wigner matrices are used as a basis set for an expansion of the orientation–distribution function.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 371

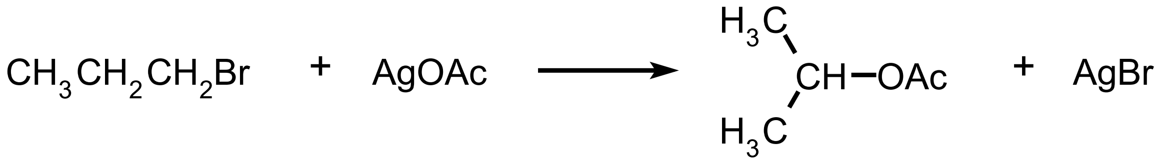
molecular rearrangement

Also contains definition of: principle of minimum structural change

The term is traditionally applied to any reaction that involves a change of connectivity (sometimes including hydrogen), and violates the so-called 'principle of minimum structural change'. According to this oversimplified principle, chemical species do not isomerize in the course of a transformation, e.g. substitution, or the change of a functional group of a chemical species into a different functional group is not expected to involve the making or breaking of more than the minimum number of bonds required to effect that transformation. For example, any new substituents are expected to enter the precise positions previously occupied by displaced groups. The simplest type of rearrangement is an intramolecular reaction in which the product is isomeric with the reactant (one type of 'intramolecular isomerization'). An example is the first step of the Claisen rearrangement:



The definition of molecular rearrangement includes changes in which there is a migration of an atom or bond (unexpected on the basis of the principle of minimum structural change), as in the reaction:

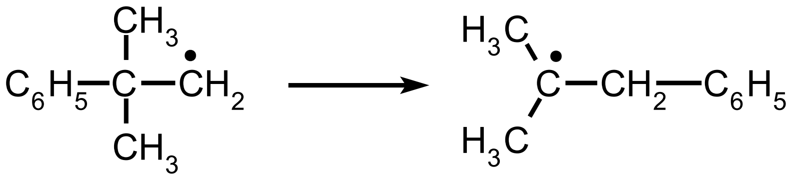


$$CH_3CH_2CH_2Br + AgOAc \longrightarrow (H_3C)_2CH{-}OAc + AgBr$$

where the rearrangement stage can formally be represented as the '1,2-shift' of hydride between adjacent carbon atoms in the carbocation:

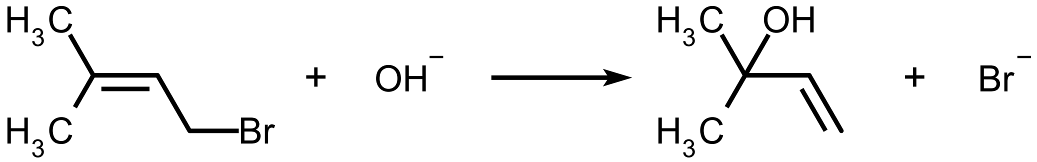
$$CH_3CH_2\overset{+}{C}H_2 \longrightarrow CH_3\overset{+}{C}HCH_3$$

Such migrations occur also in radicals, e.g.:

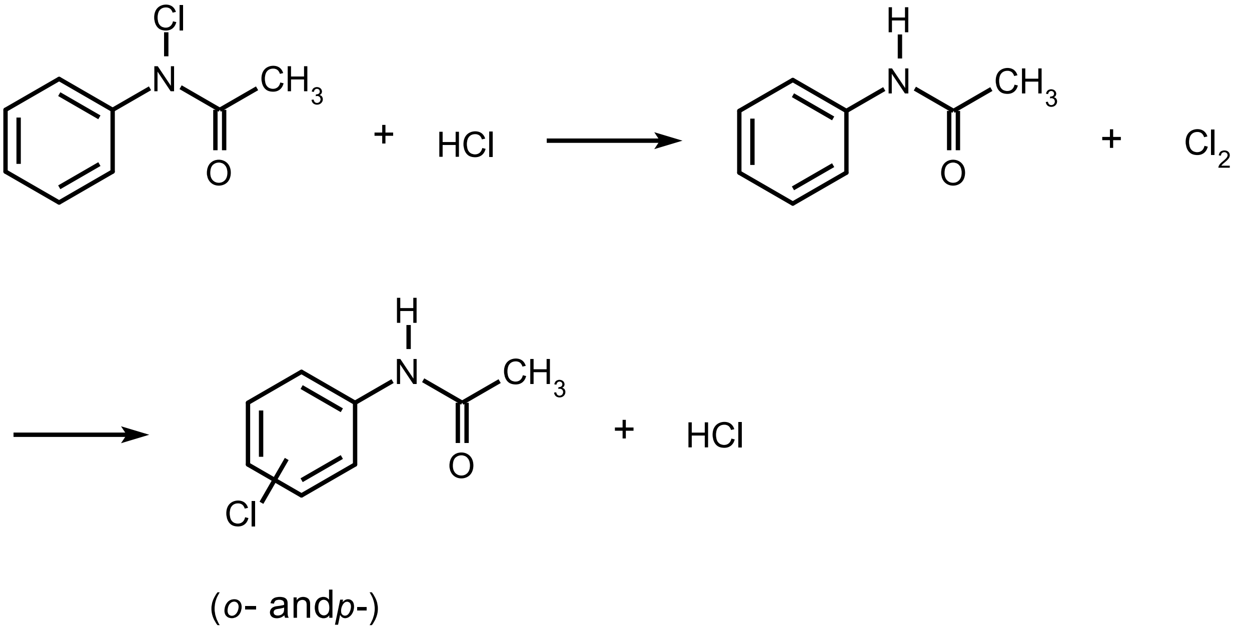


$$C_6H_5{-}C(CH_3)_2{-}\dot{C}H_2 \longrightarrow (H_3C)_2\dot{C}{-}CH_2{-}C_6H_5$$

The definition also includes reactions in which an entering group takes up a different position from the leaving group, with accompanying bond migration. An example of the latter type is the 'allylic rearrangement':



A distinction is made between 'intramolecular rearrangements' (or 'true molecular rearrangements') and ' intermolecular rearrangements' (or 'apparent rearrangements'). In the former case the atoms and groups that are common to a reactant and a product never separate into independent fragments during the rearrangement stage (i.e. the change is intramolecular), whereas in an 'intermolecular rearrangement' a migrating group is completely free from the parent molecule and is re-attached to a different position in a subsequent step, as in the Orton reaction:



Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1142

molecular Rydberg state

An excited electronic state which is composed primarily of atomic orbitals with principal quantum numbers greater than that of the ground state and the valence excited states. Such electronic states typically have a large polarizability.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1952

molecular shape

The molecular shape is an attribute of a molecule dealing with spatial extension, form, framework, or geometry. It is often described by, *e.g.*, principal axes, ovality, or connectivity indices.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1147

molecular sieve effect

With respect to porous solids, the surface associated with pores communicating with the outside space may be called the internal surface. Because the accessibility of ores may depend on the size of the fluid molecules, the extent of the internal surface may depend on the size of the molecules comprising the fluid, and may be different for the various components of a fluid mixture. This effect is known as the molecular sieve effect.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 585

molecular spectra

Spectra formed by bands consisting of rotational lines originating from rotational, vibrational and electronic transitions of molecules. These may be emission or absorption spectra.

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1461

molecular weight

See: relative molecular mass

Source:
Green Book, 2nd ed., p. 41
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 983

molecular-weight exclusion limit

in polymers

See: molar-mass exclusion limit

Source:
Purple Book, p. 69

molecularity

Also contains definitions of: bimolecular, termolecular, unimolecular

The number of reactant molecular entities that are involved in the 'microscopic chemical event' constituting an elementary reaction. (For reactions in solution this number is always taken to exclude

molecular entities that form part of the medium and which are involved solely by virtue of their solvation of solutes.) A reaction with a molecularity of one is called 'unimolecular', one with a molecularity of two 'bimolecular' and of three 'termolecular'.
See also: chemical reaction, order of reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1143
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 175
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2296

molecule

An electrically neutral entity consisting of more than one atom ($n > 1$). Rigorously, a molecule, in which $n > 1$ must correspond to a depression on the potential energy surface that is deep enough to confine at least one vibrational state.
See also: molecular entity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1143

molfile

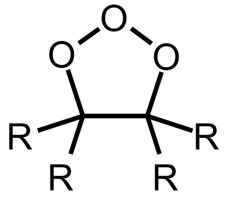
A molfile is a table containing atom type, connectivity and a more or less arbitrary *2D* or *3D* information about a molecule. Well-known file formats include the MOLfile used by MDL Information Systems Inc. (*e.g.*, in the database MACCS), the MOL2 file used by Tripos Associates (*e.g.*, in the modeling package SYBYL), or the CSSR format.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1147

See also:
MOL file format
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1146

molozonides

1,2,3-Trioxolanes, the primary products of the reaction of ozone at a carbon–carbon double bond.



See: ozonides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1349

moment of a force, *M*

About a point is the vector product of the radius vector from this point to a point on the line of action of the force and the force, $\boldsymbol{M} = \boldsymbol{r} \times \boldsymbol{F}$.

Source:
Green Book, 2nd ed., p. 12
ISO 31-2: 1992 *(Quantities and Units - Part 2: Periodic and Related Phenomena.)*

moment of inertia, *I*, *J*

Of a body about an axis is the sum of the products of its mass elements and the squares of their distances to the axis. Principal moments of inertia of a molecule are chosen so that $I_A \le I_B \le I_C$.

Source:
Green Book, 2nd ed., p. 12
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 983

momentum, *p*

Vector quantity equal to the product of mass and velocity.

Source:
Green Book, 2nd ed., p. 12

momentum spectrum

A spectrum which is obtained when a beam of ions is separated according to the momentum-to-charge ratios of the ionic species contained within it. A sector magnetic field achieves separation of the various ionic species in this way. If the ion beam is homogeneous in translational energy, as is the case with sector instruments, separation according to the $\frac{m}{z}$ ratios is also achieved and a mass spectrum is obtained.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1551

monitoring

Continuous or repeated observation, measurement, and evaluation of health and/or environmental or technical data for defined purposes, according to prearranged schedules in space and time, using comparable methods for sensing and data collection.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1061

mono-energetic radiation

Radiation consisting of particles of a single kinetic energy or photons of a single energy.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

monochromator

Optical device that transmits a mechanically selectable narrow band of wavelengths of electromagnetic radiation chosen from a wider range of wavelengths available at the input.
Note:
To spatially separate the wavelengths, a monochromator can use either the phenomenon of optical dispersion in a prism, or that of diffraction using a grating.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 372

monoclonal antibodies (MAbs)

A single species of immunoglobulin molecules produced by culturing a single clone of a hybridoma cell. MAbs recognize only one chemical structure, i.e. they are directed against a single epitope of the antigenic substance used to raise the antibody.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 161

monodisperse medium

A colloidal system in which all particles are of (nearly) the same size.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

monodisperse polymer

See: uniform polymer

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2301

monoisotopic mass spectrum

A spectrum containing only ions made up of the principal isotopes of atoms making up the original molecule.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1556

monolayer

Also contains definition of: floating monolayer

A single, closely packed layer of atoms or molecules. The term floating monolayer is used for certain spread monolayers or films which are in the condensed — often solid — state. The term Langmuir monolayer has recently been coined for spread monolayers. This usage is not recommended.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1672

See also:
Orange Book, p. 251

monolayer capacity

For chemisorption the amount of adsorbate which is needed to occupy all adsorption sites as determined by the structure of the adsorbent and by the chemical nature of the absorptive. For physisorption, the amount needed to cover the surface with a complete monolayer of atoms or molecules in close-packed array, the kind of close packing having to be stated explicitly when necessary.

Source:
Orange Book, p. 252
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 587

PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 75

monolith

Shaped, fabricated, intractable article with a homogeneous microstructure which does not exhibit any structural components distinguishable by optical microscopy.
Note:
The article is usually fabricated by cold pressing or hot pressing of a polymeric material, or by using a reactive processing technique such as reaction injection moulding, crosslinking, sol-gel processing, sintering, *etc*.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1812

monomer

A substance composed of monomer molecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2290

monomer molecule

A molecule which can undergo polymerization thereby contributing constitutional units to the essential structure of a macromolecule.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2289

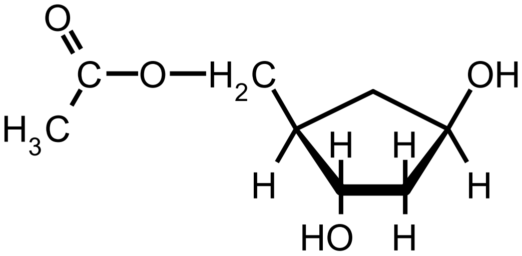
monomeric unit (monomer unit, mer)

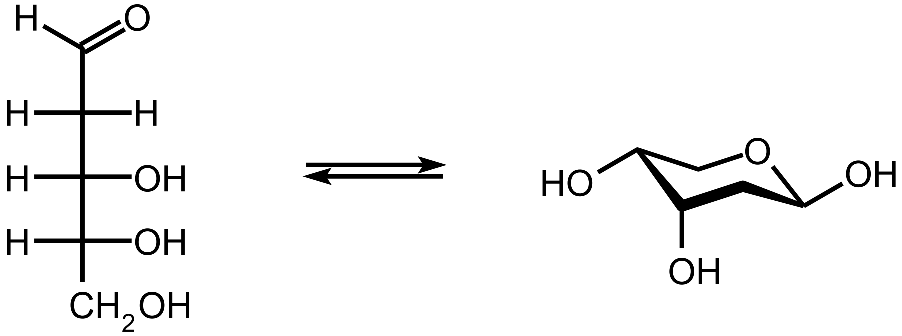
The largest constitutional unit contributed by a single monomer molecule to the structure of a macromolecule or oligomer molecule.
Note:
The largest constitutional unit contributed by a single monomer molecule to the structure of a macromolecule or oligomer molecule may be described as either monomeric, or by monomer used adjectivally.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2290

monosaccharides

A term which includes aldoses, ketoses and a wide variety of derivatives. Derivation includes oxidation, deoxygenation, introduction of other substituents, alkylation and acylation of hydroxy groups, and chain branching. E.g.





See also: aldoketoses, uronic acids, amino sugars, saccharides, glycosides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1349

monotectic reaction

The reversible transition, on cooling, of a liquid to a mixture of a second liquid and a solid:

$$\text{liquid}_1 \rightleftarrows \text{liquid}_2 + \text{ solid}.$$

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 586

monotectoid reaction

A reaction in a system containing two solid solution phases, $\alpha^{'}$ and $\alpha^{''}$ in which $\alpha^{'}$ decomposes into $\alpha^{''}$ and a new phase β:

$$\alpha^{'} \rightleftharpoons \alpha^{''} + \beta$$

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 586

monotectoid temperature

The maximum temperature at which a monotectoid reaction can occur.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 586

monoterpenoids

Terpenoids having a C_{10} skeleton.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1349

monotropic transition

The irreversible transition from a metastable polymorphic form to the stable polymorph. Example: The transition of metastable $CaCO_3$ (aragonite-type) to the stable $CaCO_3$ (calcite-type).
Note:
For liquid crystals the term refers to a liquid crystal to liquid-crystal transition that occurs below the melting point and is revealed by supercooling of the crystal.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 586

Monte Carlo (MC), method of

In mathematics, a method originally used for calculating multiple integrals by means of a random sample. The method is used for numerical modelling of many-particle chemical systems, in particular liquids; it is based on the equilibrium statistical mechanics theory. Observables A are calculated as mean values over a great number ($\cong 10^5 - 10^6$) of instant configurations as determined by coordinates of the particles.

$$< A > = \frac{1}{N} \sum_{i=1}^{N} A\{r_i\}$$

where N is the number of configurations. At the first stage, various configurations are randomly generated and then those energetically un-realizable eliminated. An efficient search for the most probable configurations to be entered into the above expression is provided by the Metropolis algorithm based on the principle of Markov's chain theory. While being elaborated for the study of equilibrium chemical systems, MC method is also applied to studies of the dynamics of chemical reactions.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1952

Monte Carlo study

Simulation and analysis of a sequence of events using random numbers to generate possible outcomes in an iterative process.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1061

mordant

Substance that fixes a dyestuff in or on a material by combining with the dye to form an insoluble compound, used to fix or intensify stains in a tissue or cell preparation.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2072

More O'Ferrall–Jencks diagram

Visualization of the potential energy surfaces for a reacting system, as a function of two chosen coordinates. It is particularly useful to discuss structural effects on the transition state geometry for processes occurring either by stepwise or concerted routes. The use of such diagrams, first suggested for elimination reactions, was later extended to acid–base catalysis and to certain other reactions.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1143

Morin transition

Synonym: spin-flop transition

A transition specific to α-Fe_2O_3 in which there is a change in the direction of the atomic magnetic moments in the antiferromagnetic state from parallel to perpendicular to the *c*-axis. Synonymous with spin-flop transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 587

morphology

Shape, optical appearance, or form of phase domains in substances, such as high polymers, polymer blends, composites, and crystals.
Note:
For a polymer blend or composite, the morphology describes the structures and shapes observed, often by microscopy or scattering techniques, of the different phase domains present within the mixture.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2001

morphology coarsening

Also contains definition of: phase ripening

Process by which phase domains increase in size during the aging of a multiphase material.
Notes:

1. In the coarsening at the late stage of phase separation, volumes and compositions of phase domains are conserved.
2. Representative mechanisms for coarsening at the late stage of phase separation are: (1) material flow in domains driven by interfacial tension (observed in a co-continuous morphology), (2) the growth of domain size by evaporation from smaller droplets and condensation into larger droplets, and (3) coalescence (fusion) of more than two droplets. The mechanisms are usually called (1) Siggia s mechanism, (2) Ostwald ripening (or the Lifshitz–Slyozov mechanism), and (3) coalescence.
3. Morphology coarsening can be substantially stopped by, for example, vitrification, crosslinking, and **pinning**, the slowing down of molecular diffusion across domain interfaces.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2000

morphotropic transition

An abrupt change in the structure of a solid solution with variation in composition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 587

Morse potential

The empirical function relating the potential energy of a molecule to the inter-atomic distance r accounting for the anharmonicity (***See:*** harmonic approximation) of bond stretching:

$$E(r) = D_{\mathrm{e}}\,(1 - \mathrm{e}^{-a\,(r-r_{\mathrm{e}})})^2$$

where D_e is the bond-dissociation energy, r_e is the equilibrium bond length, and a is a parameter characteristic of a given molecule.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1953

Mössbauer effect

Resonance absorption of γ-radiation by nuclei arranged in a crystal lattice in such a way that the recoil momentum is shared by many atoms.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

Mössbauer thickness

in Mössbauer spectroscopy

The effective thickness of a source (t_s) or absorber (t_a) in the optical path.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 214

most probable distribution (in macromolecular assemblies)

A discrete distribution with the differential mass-distribution function of the form:

$$f_w(x) = a^2\, x\, (1 - a)^{x-1}$$

where x is a parameter characterizing the chain length, such as relative molecular mass or degree of polymerization and a is a positive adjustable parameter. For large values of x, the most probable distribution converges to the particular case of the Schulz–Zimm distribution with $b = 1$. In the literature, this distribution is sometimes referred to as the Flory distribution or the Schulz–Flory distribution.

Source:
Purple Book, p. 56

Mott transition

Synonym: Mott–Hubbard transition

A transition occurring only in 'single-valent' systems from strongly correlated ($U > W$) to weakly correlated ($U < W$) electrons as a result of a change of bandwidth W. W reflects the strength of the interatomic interactions in a periodic array of like atoms and U is a measure of the intra-atomic interactions, i.e. the electrostatic energy involved in the creation of polar states by transferring an electron from one atom to the next, as shown schematically by the disproportionation reaction:

$$\mathrm{M}^{n+} + \mathrm{M}^{n+} \rightarrow \mathrm{M}^{(n+1)+} + \mathrm{M}^{(n-1)+}$$

A $U > W$ produces a magnetic semiconductor; a $U < W$ gives rise to a metal (normally nonmagnetic). Note also that U and W can be altered by changes in interatomic distances, brought about through temperature or pressure variations or by introducing an alloying element. Synonymous with Mott–Hubbard transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 587

mucopolysaccharides

Polysaccharides composed of alternating units from uronic acids and glycosamines, and commonly partially esterified with sulfuric acid.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350

See also:
White Book, p. 86

Mulliken population analysis (MPA)

A partitioning scheme based on the use of density and overlap matrixes of allocating the electrons of a molecular entity in some fractional manner among its various parts (atoms, bonds, orbitals). As with other schemes of partitioning the electron density in molecules, MPA is arbitrary and strongly dependent on the particular basis set employed. However, comparison of population analyses for a series of molecules is useful for a quantitative description of intra-molecular interactions, chemical reactivity and structural regularities.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1953

multi-centre bond

Representation of some molecular entities solely by localized two-electron two-centre bonds appears to be unsatisfactory. Instead, multi-centre bonds have to be considered in which electron pairs occupy orbitals encompassing three or more atomic centres. Examples include the three-centre bonds in diborane, the delocalized π-bonding of benzene and bridged carbocations.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1144

multi-centre reaction [obsolete]

A synonym for pericyclic reaction. The number of 'centres' is the number of atoms not bonded initially, between which single bonds are breaking or new bonds are formed in the transition state. This number does not necessarily correspond to the ring size of the transition state for the pericyclic reaction. Thus, a Diels–Alder reaction is a 'four-centre reaction'. This terminology has largely been superseded by the more detailed one developed for the various pericyclic reactions.
See: cycloaddition, sigmatropic rearrangement

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1144

multi-channel pulse height analyser

A pulse amplitude analyser which includes a storage function to record the number of pulses received per channel.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

multi-strand chain
Also contains definition of: *n*-strand chain

in polymers

A chain that comprises constitutional units connected in such a way that adjacent constitutional units are joined to each other through more than four atoms, more than two on at least one side of each constitutional unit.
Note:
A chain that comprises constitutional units joined to each other through n atoms on at least one side of each constitutional unit is termed an *n*-strand chain, e.g. three-strand chain. If an uncertainty exists in defining n, the highest possible number is selected.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2295

multi-strand macromolecule

Also contains definition of: *n*-strand molecule

A macromolecule that comprises constitutional units connected in such a way that adjacent constitutional units are joined to each other through more than four atoms, more than two on at least one side of each constitutional unit.
Note:

A macromolecule that comprises constitutional units joined to each other through n atoms on at least one side of each constitutional unit is termed an *n*-strand macromolecule, e.g. three-strand macromolecule. If an ambiguity exists in defining n, the highest possible number is selected.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2296

multicoat morphology

Morphology observed in a blend of a block copolymer with the homopolymer of one of the blocks and characterized by alternating concentric shells of the copolymer and the homopolymer.
Note:
The morphology is identical to onion morphology within a matrix of homopolymer.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2004

multiconfiguration SCF method

Also contains definition of: MCSCF method

Configuration-interaction method in which simultaneous optimization of both the shapes of molecular orbitals and contributions from different electronic configurations is carried out by using the variational method.
Note:
The MCSCF method with a large enough set of configurations allows a better estimation of the non-dynamic correlation energy than the conventional CIS, CID, and CISD methods.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 372

multienzyme

A protein possessing more than one catalytic function contributed by distinct parts of a polypeptide chain ('domains'), or by distinct subunits, or both.

Source:
White Book, p. 107

multienzyme complex

A multienzyme with catalytic domains on more than one type of polypeptide chain.

Source:
White Book, p. 107

multienzyme polypeptide

A polypeptide chain containing at least two types of catalytic domains.

Source:
White Book, p. 107

multilayer

A system of adjacent layers or monolayers. The term bilayer applies to the particular case of a multilayer two monolayers thick. Monolayers and multilayers may be alternatively named 'films' provided boundaries can be defined for them.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1672

multilayer adsorption

Adsorption such that the adsorption space accommodates more than one layer of molecules, and not all adsorbed molecules are in contact with the surface layer of the adsorbent .

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 587
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 75

multilayer aggregate

in polymer crystals

A stack of lamellar crystals generated by spiral growth at one or more screw dislocations. The axial displacement over a full turn of the screw (Burgers vector) is usually equal to one lamellar thickness.

Source:
Purple Book, p. 82

multiphase copolymer

Copolymer comprising phase-separated microdomains.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1812

multiphoton absorption

See: multiphoton process
See also: biphotonic excitation

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2255

multiphoton ionization

in mass spectrometry

Occurs when an atom or molecule and their concomitant ions have energy states whereby the energy in two or more photons is absorbed.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548

multiphoton process

A process involving interaction of two or more photons with a molecular entity.
See: biphotonic process, two-photon process

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2255

multiple inclusion morphology

Also contains definition of: salami-like morphology

Multiphase morphology in which dispersed phase domains of one polymer contain and completely encapsulate many phase domains of a second polymer that may have the same composition as the continuous phase domain.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2005

multiple peak scanning

in mass spectrometry

An alternative to multiple ion detection which emphasizes that monitoring of peaks rather than detection of ions is the important feature.

Source:
PAC, 1978, *50*, 65 *(Recommendations for symbolism and nomenclature for mass spectroscopy)* on page 69

multiple scattering

Successive rescattering of radiation within the scattering medium.
See also: light scattering

Source:
PAC, 1983, *55*, 931 *(Definitions, terminology and symbols in colloid and surface chemistry. Part 1.14: Light scattering (Provisional))* on page 932

multiple-pass cell

in spectrochemical analysis

Permits multiple passage of radiation to increase the absorption pathlength. It is constructed in such a way that mirrors either form part of the cell or are mounted in the sample cell holder.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1454

multiplex spectrometer

A spectrometer in which a single photodetector simultaneously receives signals from different spectral bands which are specifically encoded. In the case of frequency multiplexing, each spectral band is modulated at a specific frequency. Decoding is achieved by filtering out, by electronic means, the corresponding signals. Frequency multiplexing may be realized by changing the path difference between the two interfering beams at a uniform rate. Fourier transform of the interferogram so obtained yields the spectrum. This method is called Fourier transform spectrometry (FTS).

Source:
PAC, 1995, *67*, 1725 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-IX. Instrumentation for the spectral dispersion and isolation of optical radiation (IUPAC Recommendations 1995))* on page 1729

multiplicative name

A name that expresses the multiple occurrence of identical parent structures, two or more of which are connected by a symmetrical structure expressible by means of a multivalent simple or composite prefix.

Source:
Blue Book (Guide), p. 17

multiplicity (spin multiplicity)

The number of possible orientations, calculated as $2\,S+1$, of the spin angular momentum corresponding to a given total spin quantum number (S), for the same spatial electronic wavefunction. A state of singlet multiplicity has $S=0$ and $2\,S+1=1$. A doublet state has $S=\frac{1}{2}$, $2\,S+1=2$, etc. Note that when $S > L$ (the total orbital angular momentum possible) there are only $2L + 1$ orientations of total angular momentum possible.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2255

multiply labelled

A selectively labelled compound may be multiply labelled when in the unmodified compound there is more than one atom of the same element at the position where the isotopic modification occurs, e.g. H in CH_4, or there are several atoms of the same element at different positions where the isotopic modification occurs, e.g. C in C_4H_8O.

Source:
Blue Book, p. 515
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1893

multipole line

in X-ray spectroscopy

See: selection rule

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 738

multireference configuration interaction

Acronym: MRCI

Configuration-interaction method in which the configurations are built by excitation out of a wavefunction obtained by using, e.g., the multiconfiguration SCF method.
Note:
One of the methods to account for dynamic correlation.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 373

multistage sampling

Samples taken in a series of steps with the sampling portions constituting the sample (units or increments) at each step being selected from the larger or greater number of portions of the previous step, or from a primary or composite sample. The first set of portions (units or increments) taken from the population available for sampling is the primary sample. The subsequent samples (secondary, tertiary, etc.) are the sets of subsamples, units, items, individuals or increments taken from the preceding step. The units may be different steps of multistage sampling (e.g. pallets, cases, packages).

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1203

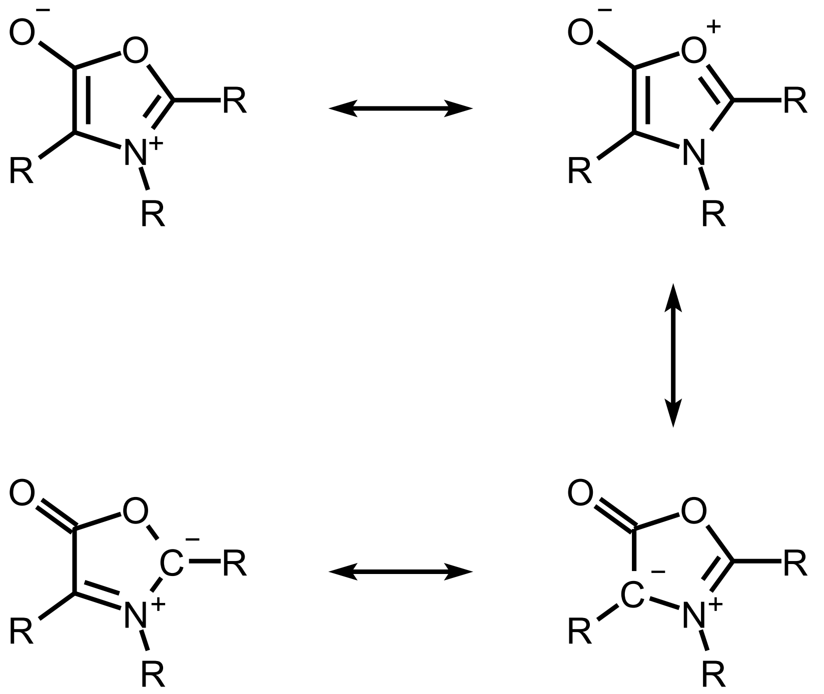
multivariate statistics

Multivariate statistics is a set of statistical tools to analyze data (*e.g.*, chemical and biological) matrices using regression and/or pattern recognition techniques.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1148

munchnones

Mesoionic compounds having a 1,3-oxazole skeleton bearing an oxygen atom attached to the 5-position with the following delocalized structure:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350

muonium

Atom-like particle consisting of a positive muon and an electron.

Source:
Green Book, 2nd ed., p. 93

mustard oils **[obsolete]**

An archaic term for isothiocyanates, RN=C=S.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350

mustards

Also contains definition of: nitrogen mustards

Compounds having two β-haloalkyl groups bound to a sulfur atom, as in $(XC_2H_2C_2H_2)_2S$, and their analogues, the nitrogen (and phosphorus) mustards, $(XC_2H_2C_2H_2)_2NR$. Compounds having one β-haloalkyl group and one β-hydroxyalkyl group on S are termed hemi- or semi-mustards by some chemists.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350

mutagen

Agent that can induce heritable changes (mutations) of the genotype in a cell as a consequence of alterations or loss of genetic material.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1062

mutagenesis

The introduction of permanant heritable changes i.e. mutations into the DNA of an organism.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 161

mutarotation

The change in optical rotation accompanying epimerization. In sugar chemistry this term usually refers to epimerization at the hemiacetal carbon atom.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

mutation

A heritable change in the nucleotide sequence of genomic DNA (or RNA in RNA viruses), or in the number of genes or chromosomes in a cell, which may occur spontaneously or be brought about by chemical mutagens or by radiation (induced mutation).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 161

mutation rate

in biotechnology

The frequency (h^{-1}) with which a mutation occurs within a organism or gene. In general, rates of spontaneous mutation vary between one in 10^4 and one in 10^8 per gene per generation, and can be considerably increased by mutagens.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 161

mutual inductance, M

For two thin conducting loops, the magnetic flux through one loop, caused by an electric current in the other loop, divided by that current.

Source:
Green Book, 2nd ed., p. 15
ISO 31-4: 1992

Myelin cylinders

Birefringent cylinders which form spontaneously from lipid-containing material in contact with water.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

n → π* state

An excited state related to the ground state by a n → π* transition.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2255

n → π* transition

An electronic transition described approximately as promotion of an electron from a 'non-bonding' (lone-pair) n orbital to an 'antibonding' π orbital designated as π*.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2255

n → σ* transition

An electronic transition described approximately as promotion of an electron from a 'non-bonding' (lone-pair) n orbital to an 'antibonding ' σ orbital designated as σ*. Such transitions generally involve high transition energies and appear close to or mixed with Rydberg transitions.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2255

n-σ* delocalization (or n-σ* no bond resonance)

Delocalization of a free electron pair (n) into an antibonding σ-orbital (σ*).
See: hyperconjugation, resonance

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1146

nano

SI prefix for 10^{-9} (symbol: n).

Source:
Green Book, 2nd ed., p. 74

nanocomposite

Composite in which at least one of the phase domains has at least one dimension of the order of nanometres.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1813

nanodomain morphology

Morphology consisting of phase nanodomains.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2004

nanofiltration

Pressure-driven membrane-based separation process in which particles and dissolved macromolecules smaller than $2\ \mathrm{nm}$ are rejected.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1487

nanogel

Also contains definition of: gel nanoparticle

Particle of gel of any shape with an equivalent diameter of approximately 1 to $100\ \mathrm{nm}$.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1807

nanoscopic film

A film which has lateral dimensions in the range of $0.1 - 100\ \mathrm{nm}$.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1671

naphthenes **[obsolete]**

Cycloalkanes especially cyclopentane, cyclohexane and their alkyl derivatives. The term seems to be obsolescent, except in the petrochemical industry.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350

naphthenic acids **[obsolete]**

Acids chiefly monocarboxylic, derived from naphthene. The term seems to be obsolescent, except in the petrochemical industry.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350

narcissistic reaction [obsolete]

A chemical reaction that can be described as the conversion of a reactant into its mirror image, without rotation or translation of the product, so that the product enantiomer actually coincides with the mirror image of the reactant molecule. Examples of such reactions are cited under the entries fluxional and degenerate rearrangement.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1144

natural atomic orbital (NAO)

A valence-shell atomic orbital whose derivation involves diagonalising the localized block of the full density matrix of a given molecule associated with basis functions $\chi_i(\mathrm{A})$ on that atom. A distinguishing feature of NAOs is that they meet the simultaneous requirement of orthonormality and maximum occupancy. For isolated atoms, NAOs coincide with natural orbitals. In a polyatomic molecule the NAOs (in contrast to natural orbitals that become delocalised over all nuclear centres) mostly retain one-centre character, and thus are optimal for describing the molecular electron density around each atomic centre.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1954

natural bond orbital (NBO)

The orbital which is formed from natural hybrid orbitals. For a localized σ-bond between atoms A and B, the NBO is:

$$\sigma_{\mathrm{AB}} = c_{\mathrm{A}}\,\mathrm{h}_{\mathrm{A}} + c_{\mathrm{B}}\,\mathrm{h}_{\mathrm{B}}$$

where h_{A} and h_{B} are the natural hybrids centred on atoms A and B. NBOs closely correspond to the picture of localized bonds and lone pairs as basic units of molecular structure, so that is possible to conveniently interpret *ab initio* wave-functions in terms of the classical Lewis structure concepts by transforming these functions to NBO form.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1954

natural broadening

of a spectral line

Broadening which has its origin in the finite optical lifetime of one or both levels involved in the transition.

Source:
Orange Book, p. 121
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1463

natural graphite

A mineral found in nature. It consists of graphitic carbon regardless of its crystalline perfection.
Note:
Some natural graphites, often in the form of large flakes, show very high crystalline perfection. Occasionally, they occur as single crystals of graphite. The use of the term natural graphite as a synonym for the term 'graphite single crystal' is incorrect and should be avoided. Varieties of natural graphite with lower structural perfection are classified as 'microcrystalline natural graphite'. Commercial natural graphite is often contaminated with other minerals, e.g. silicates, and may contain rhombohedral graphite due to intensive milling.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 497

natural hybrid orbital (NHO)

Symmetrically orthogonalised directed hybrid orbital derived through unitary transformation of natural atomic orbitals centred on a particular atom.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1954

natural isotopic abundance

Of a specified isotope of an element, the isotopic abundance in the element as found in nature.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

natural orbital

The orbitals defined (P. Lowdin) as the eigenfunctions of the spinless one-particle electron density matrix. For a configuration interaction wave-function constructed from orbitals Φ, the electron density function, ρ, is of the form:

$$\rho = \sum_{i}\sum_{j} a_{ij}\, \Phi_i^* \,\Phi_j$$

where the coefficients a_{ij} are a set of numbers which form the density matrix. The NOs reduce the density matrix ρ to a diagonal form:

$$\rho = \sum_{k} b_k\, \Phi_k^* \,\Phi_k$$

where the coefficients b_k are occupation numbers of each orbital. The importance of natural orbitals is in the fact that CI expansions based on these orbitals have generally the fastest convergence. If a CI calculation was carried out in terms of an arbitrary basis set and the subsequent diagonalisation of the density matrix a_{ij} gave the natural orbitals, the same calculation repeated in terms of the natural orbitals thus obtained would lead to the wave-function for which only those configurations built up from natural orbitals with large occupation numbers were important.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1954

natural population analysis (NPA)

The analysis of the electron density distribution in a molecular system based on the orthonormal natural atomic orbitals. Natural populations, $n_i(\mathrm{A})$ are the occupancies of the natural atomic orbitals. These rigorously satisfy the Pauli exclusion principle: $0 < n_i(\mathrm{A}) < 2$. The population of an atom $n(\mathrm{A})$ is the sum of natural populations $n(\mathrm{A}) = \sum_{\mathrm{A}} n_i(\mathrm{A})$. A distinguished feature of the NPA method is that it largely resolves the basis set dependence problem encountered in the Mulliken population analysis method.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1954

natural radiation

Radiation originating from natural radioactivity.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1549

natural radioactivity

Radioactivity of naturally occurring nuclides in materials where the isotopic abundance of that nuclide is natural.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

necrosis

Sum of morphological changes resulting from cell death by lysis and/or enzymatic degradation, usually affecting groups of cells in a tissue.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1062

needle coke

The commonly used term for a special type of coke with extremely high graphitizability resulting from a strong preferred parallel orientation of its turbostratic layer structure and a particular physical shape of the grains.
Note:
Needle coke is derived mainly from clean (i.e. lacking hetero atoms and solids) and highly aromatic (i.e. several condensed rings per cluster) feedstocks with a very low concentration of insolubles. Upon solidification a material with a distinctive streaked or flow-like macroscopic appearance is produced. Upon grinding the coke breaks up first into macroscopic needles and then, after further grinding, into microplatelets. Sometimes the word 'acicular' is used as a synonym for needle-like.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 497

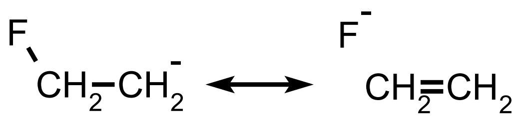
negative adsorption

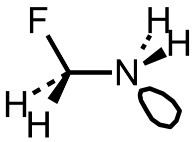
The depletion of one or more components in an interfacial layer.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 584

negative hyper-conjugation

The effect of donation of electron density from filled π or n_π-orbitals to the symmetry adapted σ^*-orbital(s) of σ-bond(s) of a molecular entity resulting in building π-character into bonds that nominally possess only σ-character. The consequences of the effect are, for example, in elongation of the C–F bond in the β-fluoroethyl anion and stabilization of the anti-periplanar conformation of fluoromethylamine.





Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1954

negative ion

in mass spectrometry

An atom, radical, molecule or molecular moiety in the vapour phase which has gained one or more electrons thereby acquiring an electrically negative charge. The use of the term anion as an alternative is not recommended because of its connotations in solution chemistry.
See: positive ion

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549
Orange Book, p. 204

negaton

See: electron

Source:
Orange Book, p. 221

neighbouring group participation

Also contains definitions of: anchimeric assistance, synartetic acceleration

The direct interaction of the reaction centre (usually, but not necessarily, an incipient carbenium centre) with a lone pair of electrons of an atom or with the electrons of a σ- or π-bond contained within the parent molecule but not conjugated with the reaction centre. A distinction is sometimes made between n-, σ- and π-participation. A rate increase due to neighbouring group participation is known as 'anchimeric assistance'. 'Synartetic acceleration' is the special case of anchimeric assistance ascribed to participation by electrons binding a substituent to a carbon atom in a β-position relative to the leaving group attached to the α-carbon atom. According to the underlying model, these electrons then provide a three-centre bond (or 'bridge') 'fastening together' (as the word 'synartetic' is intended to suggest) the α- and β-carbon atoms between which the charge is divided in the intermediate bridged ion formed (and in the transition state preceding its formation). The term synartetic acceleration is not widely used.
See also: intramolecular catalysis, multi-centre bond

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1145

neodymium laser

Also contains definition of: YAG

A CW pulsed laser emitting radiation from excited Nd^{3+} principally occurring around $1.06\ \mu m$ (the precise position depends on the matrix). The Nd^{3+} is present as a dopant in suitable crystals (e.g. yttrium–aluminium garnet, YAG) or in suitable glasses (phosphate, silicate, etc.).
See: solid-state lasers

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2256

neper

Unit, coherent with the SI, for expressing field levels, $\mathrm{Np} = 1$.

Source:
Green Book, 2nd ed., p. 78

nephelometry

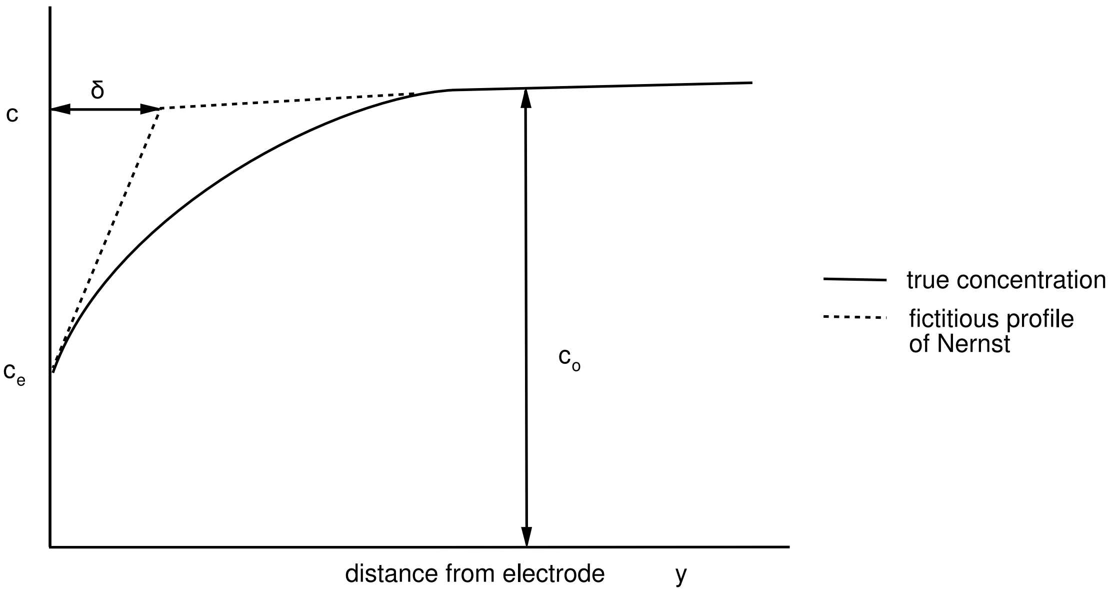
Analytical methods which depend on the measurement of the intensity of scattered light emanating from an illuminated volume of an aerosol. The ratio of scattered intensity to illuminating intensity is compared with a standard of known properties.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2202

Nernst's diffusion layer

Also contains definition of: effective thickness of diffusion layer

A fictitious layer corresponding to the dotted straight lines of the diagram which shows the concentration profile along the direction perpendicular to an electrode surface. The thickness δ of this layer is called the effective (or equivalent) thickness of the diffusion layer. Its definition is apparent from the figure. It is the thickness which the diffusion layer would have if the concentration profile were a straight line coinciding with the tangent to the true concentration profile at the interface, and that straight line were extended up to the point where the bulk concentration is reached. δ has a formal significance only. It is simply another way of writing the mass transfer coefficient k_{d} defined in terms of a resistivity instead of a conductivity.



Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1837

net current

The sum of cathodic and anodic partial currents.

Source:
PAC, 1980, *52*, 233 *(Electrode reaction orders, transfer coefficients and rate constants. Amplification of definitions and recommendations for publication of parameters)* on page 236

net electric charge, *z*

of a particle

in electrophoresis

The algebraic sum of the charges present at the surface of the particle divided by the elementary charge of the proton. The symbol z is also used for charge number of an ion.

Source:
PAC, 1994, *66*, 891 *(Quantities and units for electrophoresis in the clinical laboratory (IUPAC Recommendations 1994))* on page 895

net

in surface chemistry

A two-dimensional lattice (in a particular range of surface coverage and temperature) into which the adsorbate is ordered, especially in some cases of localized adsorption.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

net shaping

Production of an object in, or as close as possible to, its final shape prior to ceramization.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1824

network

Highly ramified structure in which essentially each constitutional unit is connected to each other constitutional unit and to the macroscopic phase boundary by many paths through the structure, the number of such paths increasing with the average number of intervening constitutional units; the paths must on average be co-extensive with the structure.
Notes:

1. Usually, and in all systems that exhibit rubber elasticity, the number of distinct paths is very high, but, in most cases, some constitutional units exist that are connected by a single path only.
2. Modified from previous definition. The definition proposed here is a generalization to cover both polymeric networks and networks comprised of particles.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1813

network defect

Elastically ineffective chains in a polymer network.
Note:
A network defect is caused by a loose end or a cyclic structure.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1820

network

Also contains definition of: covalent network

in polymer chemistry

A highly ramified macromolecule in which essentially each constitutional unit is connected to each other constitutional unit and to the macroscopic phase boundary by many permanent paths through the macromolecule, the number of such paths increasing with the average number of intervening bonds; the paths must on the average be co-extensive with the macromolecule.

Notes:

1. Usually, and in all systems that exhibit rubber elasticity, the number of distinct paths is very high, but, in most cases, some constitutional units exist which are connected by a single path only.
2. If the permanent paths through the structure of a network are all formed by covalent bonds, the term covalent network may be used.
3. The term physical network may be used if the permanent paths through the structure of a network are not all formed by covalent bonds but, at least in part, by physical interactions, such that removal of the interactions leaves individual macromolecules or a macromolecule that is not a network.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2298

network polymer

A polymer composed of one or more networks.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2305

network-chain molar mass, M_c

Also contains definition of: inter-junction molar mass

Number-average molar mass of polymer chains between two adjacent crosslinks or junction points in a polymer network.
Note:
SI units kg mol^{-1}.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1820

neutralized gel

Gel containing acidic or basic groups that have been neutralized.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1807

neutrino (electron neutrino)

An elementary particle of negligible mass and zero electric charge. There are also a muon neutrino and tau neutrino.

Source:
Green Book, 2nd ed., p. 93

neutron

Nuclear particle of zero charge, spin quantum number $\frac{1}{2}$ and a mass of $1.008\ 664\ 904(14)\ \mathrm{u}$.

Source:
Green Book, 2nd ed., p. 93

neutron density

The number of free neutrons divided by the containing volume. Partial densities may be defined for neutrons characterized by such parameters as energy and directions.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

neutron multiplication

The process in which a neutron produces on the average more than one neutron in a medium containing fissile material.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1546

neutron number, N

Number of neutrons in an atomic nucleus.

Source:
Green Book, 2nd ed., p. 20

neutron rest mass

Atomic fundamental physical constant $m_{\mathrm{n}} = 1.674\ 9286(10) \times 10^{-27}\ \mathrm{kg}$.

Source:
CODATA Bull. 1986, *63*, 1

neutron temperature

The temperature assigned to a population of neutrons when this population is approximated by a Maxwellian distribution.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

neutrophilic organisms

Organisms preferring a neutral medium for growth.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 161

Newman projection

A projection formula representing the spatial arrangement of bonds on two adjacent atoms in a molecular entity. The structure appears as viewed along the bond between these two atoms, and the bonds from them to other groups are drawn as projections in the plane of the paper. The bonds from the atom nearer to the observer are drawn so as to meet at the centre of a circle representing that atom. Those from the further atom are drawn as if projecting from behind the circle.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

newton

SI derived unit of force, $\mathrm{N} = \mathrm{kg\ m\ s^{-2}}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 984

Newton black film

In soap films, two types of equilibrium film are often observed, sometimes successively in the same system: one characterized by thicknesses of the order of $7\ \mathrm{nm}$ or more which varies significantly with minor changes in composition such as ionic strength, and the other having a lesser thickness relatively independent of such changes. When a distinction is needed, the former are designated as common black films, and the latter as Newton black films. The current use of first or secondary for the common black film and of second, primary or Perrin's for the Newton black film is discouraged.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 614

Newton diagram

A vector diagram used to show the relationship between initial and final velocities or momenta in a two-particle scattering process. It is commonly used to relate laboratory and centre-of-mass coordinates.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 175

Newtonian fluid

A fluid in which the components of the stress tensor are linear functions of the first spatial derivatives of the velocity components. These functions involve two material parameters (taken as constants throughout the fluid, although depending on ambient temperature and pressure).

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1216

nido-

An affix used in names to denote a nest-like structure, especially a boron skeleton that is almost closed.

Source:
Red Book, p. 245
Blue Book, p. 465

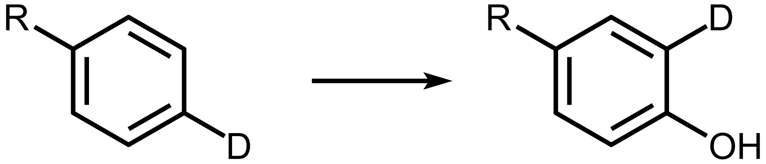
Nier–Johnson geometry

An arrangement for a double-focusing mass spectrometer in which a deflection of $\frac{\pi}{2}$ radians in a radial electrostatic field analyser is followed by a magnetic deflection of $\frac{\pi}{3}$ radians. The electrostatic analyser uses a symmetrical object-image arrangement and the magnetic analyser is used asymmetrically.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546
Orange Book, p. 201

NIH shift

The intramolecular hydrogen migration which can be observed in enzymatic and chemical hydroxylations of aromatic rings. It is evidenced by appropriate deuterium labelling, i.e.



In enzymatic reactions the NIH shift is generally thought to derive from the rearrangement of arene oxide intermediates, but other pathways have been suggested. (NIH stands for U.S. National Institutes of Health where the shift was discovered.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1145

nimbostratus cloud

in atmospheric chemistry

An amorphous, dark grey, rainy cloud layer reaching almost to the ground; $300 - 600\ \mathrm{m}$; vertical velocities of $0.05\ - 0.2\ \mathrm{m\ s^{-1}}$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

nitramines

Amines substituted at N with a nitro group (a contracted form of *N*-nitroamines); they are thus amides of nitric acid, and the class is composed of nitramide, O_2NNH_2, and its derivatives formed by substitution.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350

nitrenes

Synonym: aminylenes

1. The neutral compound HN: having univalent nitrogen, and its derivatives RN. Aminylenes is a recognized but less widely used synonym. Other names that have been used include aminediyls, imidogens, azenes. They may exist in either a singlet or a triplet electronic state (four spin-paired electrons, or two spin-paired and two with parallel spins, respectively), e.g. CH_3N: methylnitrene.
2. Until the 1960s, nitrenes had a totally different meaning: analogues of nitrones in which the double-bonded oxygen is replaced by double-bonded carbon, thus azomethine ylides.

See: carbenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350
PAC, 1993, *65*, 1357 *(Revised nomenclature for radicals, ions, radical ions and related species (IUPAC Recommendations 1993))* on page 1357

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1145

nitrenium ions

Synonym: aminylium ions

The cation ($H_2N{:}^+$) and its *N*-hydrocarbyl derivatives ($R_2N{:}^+$), in which the nitrogen has a positive charge, and two unshared electrons. A synonymous but less widely used term is aminylium ions. The alkylidene derivatives of ($H_2N{:}^+$), ($R_2C{=}N{:}^+$), still belong to the class nitrenium ions, but are more precisely designated by the term iminylium ions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1145

nitrification

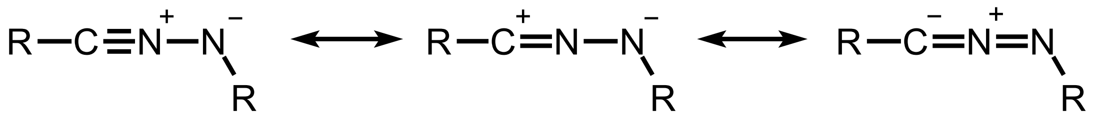
Sequential oxidation of ammonium salts to nitrite and nitrate by microorganisms.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2075

nitrile imides

Synonym: nitrilimines

Ylides having the structure



. Also known as nitrile imines or nitrilimines, especially in the German literature.
See also: dipolar compounds

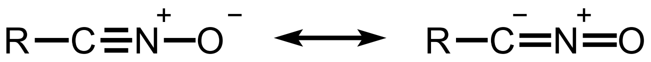
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitrile imines

See: nitrile imides, imides (2)

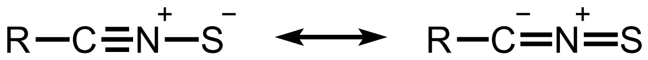
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitrile oxides

Ylides having the structure  .
See also: dipolar compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitrile sulfides

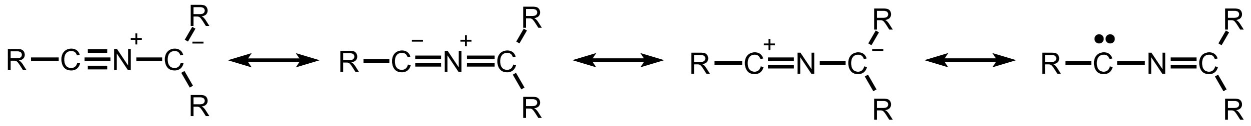
Sulfur analogues of nitrile oxides  .
See also: dipolar compounds

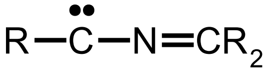
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitrile ylides

Also contains definition of: alkylideneamino carbenes

1,3-Dipolar compounds having the structure:



The uncharged canonical form  $R{-}\ddot{C}{-}N{=}CR_2$ is called an alkylidene- (or hydrocarbylidene-) amino carbene; the name iminyl carbene is incorrect because iminyl is not a recognized prefix for $–N{=}CR_2$.
See also: carbenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitriles

Compounds having the structure RC≡N; thus *C*-substituted derivatives of hydrocyanic acid, HC≡N. In systematic nomenclature, the suffix nitrile denotes the triply bound ≡N atom, not the carbon atom attached to it.
See also: cyanides, isocyanides, carbonitriles

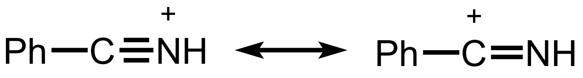
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1350

nitrilium betaines

Derivatives of nitriles having the general structure $R{-}C{\equiv}N^{+}{-}Y^{-}$. A subclass of 1,3-dipolar compounds including nitrile imides, nitrile oxides, nitrile sulfides and nitrile ylides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitrilium ions

Cations derived formally by attachment of one hydron to the nitrogen atom of a nitrile and hydrocarbyl derivatives thereof. E.g.  $Ph{-}C{\equiv}\overset{+}{N}H \longleftrightarrow Ph{-}\overset{+}{C}{=}NH$ benzonitrilium.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitrimines

Compounds having the structure $O_2NN{=}CR_2$ (also called *N*-nitroimines).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitro compounds

Compounds having the nitro group, $-NO_2$ (free valence on nitrogen), which may be attached to carbon, nitrogen (as in nitramines), or oxygen (as in nitrates), among other elements (in the absence of specification, *C*-nitro compounds are usually implied).
See also: dipolar compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitrogen fixation

The assimilation of atmospheric nitrogen by microbial reduction to ammonia and conversion into organonitrogen compounds such as amino acids. Only a limited number of microorganisms are able to fix nitrogen.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 161

nitrogen laser

A source of pulsed semi-coherent superradiance mainly around $337\ \mathrm{nm}$. The lasing species is molecular nitrogen.
See: gas lasers

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2256

nitrolic acids

Compounds having the structure $RC(=NOH)NO_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitrones

The *N*-oxides of imines, that have the structure $R_2C=N^+(O^-)R'$ ($R' \neq H$). Synonymous with azomethine oxides. *N*-Oxides $R_2C=N^+(O^-)H$ may be included.

See also: dipolar compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1351

nitrosamides

Although this term has, regrettably, been used to mean the *N*-nitroso derivatives of amides, logically it refers to amides of nitrous acid; the unstable parent compound H_2NNO is, in fact, named nitrosamide, but its derivatives formed by substitution with hydrocarbyl groups are by long custom called nitrosamines.
See also: nitramines

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

nitrosamines

N-Nitroso amines, compounds of the structure R_2NNO. Compounds RNHNO are not ordinarily isolable, but they, too, are nitrosamines. The name is a contraction of *N*-nitrosoamine and, as such, does not require the *N* locant.
See also: nitrosamides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

nitrosimines

N-Nitroso imines $O{=}NN{=}CR_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

nitroso compounds

Compounds having the nitroso group, –NO. attached to carbon, or to another element, most commonly nitrogen or oxygen.
See: nitrosamines

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

nitrosolic acids

Compounds having the structure RC(=NOH)NO.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

nitroxides

Nitroxide is the parent name used by Chemical Abstracts Service for $H_2N–O^{\cdot}$, e.g. $(ClCH_2)_2N–O^{\cdot}$ bis(chloromethyl) nitroxide. The IUPAC name is bis(chloromethyl)aminoxyl. Nitroxides should not be used as a class name for aminoxyl radicals.
See: aminoxyl radicals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

nitroxyl radicals

See: aminoxyl radicals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

no carrier added

A preparation of a radioactive isotope which is essentially free from stable isotopes of the element in question.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

no observed adverse effect level (NOAEL)

Greatest concentration or amount found by experiment or observation, which causes no detectable adverse alteration of morphology, functional capacity, growth, development, or life span of the target organism under defined conditions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2076
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1023
This definition replaces an earlier definition of no-observed-adverse-effect-level (NOAEL).

no-bond resonance

See: hyperconjugation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1145

no-load indication (for a precision balance)

The deflection or rest point (no-load reading) multiplied by the value of the division for zero load (rider at zero); symbol i_0.

Source:
Orange Book, p. 36

no-observed-effect-level (NOEL)

Greatest concentration or amount of a substance, found by experiment or observation, that causes no alterations of morphology, functional capacity, growth, development, or life span of target organisms distinguishable from those observed in normal (control) organisms of the same species and strain under the same defined conditions of exposure.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2076

nodal plane

A plane of a system in which the value of the orbital wave-function equals zero. This plane defines a region of zero electron density for the orbital.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1955

noise

The random fluctuations occurring in a signal that are inherent in the combination of instrument and method.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1663

See also:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1750

nominal linear flow, F

in chromatography

The volumetric flowrate of the mobile phase divided by the area of the cross section of the column ($\mathrm{cm\ min^{-1}}$) i.e. the linear flowrate in a part of the column not containing packing.

Source:
Orange Book, p. 102

nominally labelled tracer

A tracer in which the label is present mainly in a specified position.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

non-calorimetric thermophysical measurements

These include (p, V, T) measurements, saturated density measurements, and any other measurements which give information on the (p, V, T) surface of a fluid.

Source:
PAC, 1981, *53*, 1805 *(Assignment and presentation of uncertainties of the numerical results of thermodynamic measurements (Provisional))* on page 1818

non-crossing rule

Electronic states of the same symmetry cannot cross along a reaction coordinate.
Note:
Only applies to diatomic molecules and not to polyatomic molecules.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 374

non-crystalline electrodes

Electrodes in which a support matrix, containing an ion exchanger (either cationic or anionic), a plasticizer solvent, and possibly an uncharged, selectivity-enhancing species, forms the ion-selective membrane which is usually interposed between two aqueous solutions. The support used can be either macroporous [e.g. poly(propylene carbonate) filter, glass frit, etc.] or microporous (e.g. 'thirsty' glass or inert polymeric material such as PVC) yielding with the ion-exchanger and the solvent a 'solidified' homogeneous mixture. These electrodes exhibit a response due to the presence of the ion-exchange material in the membrane. The solvent-polymeric-membrane is an example.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2534

non-destructive activation analysis

An activation analysis procedure in which, after the irradiation, no chemical and physical operations are applied which cause a change of any properties of the sample.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1535

non-dissociative chemisorption

See: chemisorption

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 76

non-draining

An adjective describing a chain macromolecule that behaves in a hydrodynamic field as though the solvent within the domain of the macromolecule were virtually immobilized with respect to the macromolecule.

Source:
Purple Book, p. 61

non-equilibrium reaction

If the reactants in a chemical reaction are not initially present in a Boltzmann distribution the reaction is referred to as a non-equilibrium reaction.
See: equilibrium reaction

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 175

non-graphitic carbon

All varieties of solids consisting mainly of the element carbon with two-dimensional long-range order of the carbon atoms in planar hexagonal networks, but without any measurable crystallographic order in the third direction (*c*-direction) apart from more or less parallel stacking.
Note:

Some varieties of non-graphitic carbon convert on heat treatment to graphitic carbon (graphitizable carbon) but some others do not (non-graphitizable carbon).
See also: amorphous carbon

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 498

non-graphitizable carbon

A non-graphitic carbon which cannot be transformed into graphitic carbon solely by high-temperature treatment up to $3300\ \mathrm{K}$ under atmospheric pressure or lower pressure.
Note:
The term non-graphitizable is limited to the result of heat treatment without additional influence of foreign matter or neutron radiation. Non-graphitizable carbon can be transformed into graphitic carbon by a high-temperature process via intermediate dissolution in foreign matter and precipitation under high pressure or by radiation damage.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 498

non-ideal, linear chromatography

Chromatographic process, where the retention is governed by a linear distribution isotherm and normal peak-broadening takes place.
Note:
This case is commonly assumed in analytical chromatography.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1594

non-ideal, non-linear chromatography

Chromatographic process, where both isotherm curvature and other peak-broadening processes (such as diffusion) contribute to the peak shape.
Note:
This case comprises most peaks in common practice that are characterised as 'tailing' or 'fronting'.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1594

non-ideal chromatography

Chromatographic process with normal peak-broadening effects.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1593

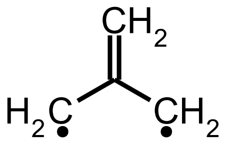
non-isotopic labelling

Labelling in which the resulting product has a different chemical composition from the initial one.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

non-Kekulé molecules

Molecules that are fully conjugated, but each of whose Kekulé structures contains at least two atoms that are not π-bonded. Examples of non-Kekule hydrocarbons are trimethylenemethane (2-methylidenepropane-1,3-diyl) **1**, *m*-benzodiquinomethane (benzene-1,2-diyldimethyl) **2**, and 1,2,4,5 - tetramethylenebenzene (benzene-1,2,4,5-tetrayltetramethyl) **3**.



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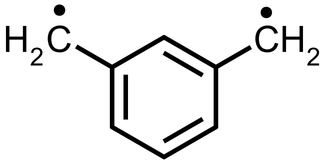

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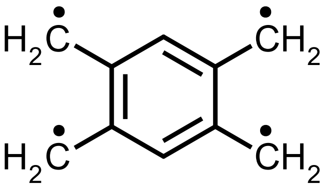

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Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1955

non-linear chromatography

Chromatographic process, where the retention is governed by a non-linear distribution isotherm.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1593

non-linear distribution isotherm

in chromatography

A distribution isotherm which is not linear.
Note:
A non-linear isotherm can have several shapes, as classified by Brunauer *et al.* In chromatography convex or concave shapes are common, as well as combinations.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1593

non-linear optical effect

An effect brought about by electromagnetic radiation the magnitude of which is not proportional to the irradiance. Non-linear optical effects of importance to photochemistry are harmonic frequency generation, lasers, Raman shifting, upconversion, and others.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2256

non-linear optical polymer

Polymer that exhibits an optical effect brought about by electromagnetic radiation such that the magnitude of the effect is not proportional to the irradiance.
Notes:
1. ***See also:*** non-linear optical effect.
2. An example of non-linear optical effects is the generation of higher harmonics of the incident light wave.
3. A polymer that exhibits a non-linear optical effect due to anisotropic electric susceptibilities when subjected to electric field together with light irradiation is called an electro-optical polymer. A polymer that exhibits electro-optical behavior combined with photoconductivity is called a photo-refractive polymer.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 900

non-linear optical techniques

Collective name applied to techniques related to non-linear optical effects.
Notes:
1. Some of these spectroscopies are four-wave mixing, hole burning, photon echoes, time-resolved coherent anti-Stokes Raman (CARS), transient grating and stimulated pumping. These techniques differ in the nature of the pulse sequence, the geometry and the choice of a spatial direction (phase matching), as well as the mode of detection.
2. Low order non-linear techniques, such as three-wave mixing, are related to the second order polarization. For a random isotropic medium with inversion symmetry, the second-order polarization vanishes and then the lowest order optical non-linear techniques, as well as the higher order non-linear techniques are related to the third-order polarization and the corresponding 'hyper-susceptibility'.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 374

non-linearity error

in spectrochemical analysis

An error caused by any deviation from linearity of the response of the detector to the measured radiant power.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1456

non-polarized interphases

Interphases for which the exchange of common charged components between the phases proceeds unhindered.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1253

non-radiative decay

The disappearance of an excited species due to a radiationless transition.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2256

non-specific adsorption

Ions approach an interface differently depending on the forces in play. Ions are non-specifically adsorbed (positively or negatively) when they are subjected in the interphase only to long-range coulombic interactions (attraction or repulsion). They are believed to retain their solvation shell, and in the position of closest approach to the interface they are separated from it by one or more molecular layers.
See also: specific adsorption

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 447

non-uniform corrosion

Corrosion is non-uniform if the time average of the corrosion current through a unit area depends on its position on the surface. Non-uniform corrosion can be due to inhomogeneities of structure or of composition of the corroding material, or to inhomogeneities of the environment. Special cases of non-uniform corrosion such as pitting or intergranular corrision are sometimes called localized corrosion.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

non-uniform polymer

A polymer comprising molecules non-uniform with respect to relative molecular mass or constitution or both.
See: uniform polymer (3)

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2302

non-vertical energy transfer

Energy transfer process with a low Franck–Condon factor because the nuclear geometries of the minima on the ground- and excited-state potential energy surfaces of the donor or of the acceptor are strongly displaced.
Note:
A Franck–Condon transition is always vertical. Thus, it is not strictly correct to speak about non-vertical transition. However, the term implies that the projection of all the vibrational wave functions of the donor state onto all the vibrational functions of the acceptor will result in low Franck–Condon factors.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 374

nonadiabatic coupling

This is momentum coupling between two adiabatic potential-energy surfaces.
See also: adiabatic

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 175

nonadiabatic electron transfer

See: diabatic electron transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2255

nonadiabatic photoreaction [obsolete]

Synonymous with diabatic photoreaction. Use of the double negative is discouraged.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2256

nonbonded interactions

Intramolecular attractions or repulsions between atoms that are not directly linked to each other, affecting the thermodynamic stability of the chemical species concerned.
See also: eclipsing strain, transannular strain

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

nonbonding molecular orbital

A molecular orbital whose occupation by electrons does not contribute (or contributes insignificantly) to the binding energy of the molecule. Generally, a nonbonding MO represents the highest occupied molecular orbital of a molecule.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1955

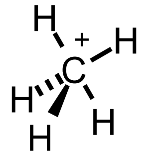
nonclassical carbocation

A carbocation the ground state of which has delocalized (bridged) bonding π- or σ-electrons. (N.B. Allylic and benzylic carbocations are not considered nonclassical.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1145

nonclassical structure

The structure of molecules or molecular ions that escapes description in terms of conventional rules of valency and stereochemistry. Nonclassical structures are characteristic of carbonium ions with hypercoordinated (see hypercoordination) carbon atoms, e.g., methanium ion **1**, pyramidal dication $C_6H_6^{2+}$ **2** (isomeric to benzene dication), and the molecular species whose structure cannot be adequately represented by the equilibrium (2-norbornyl cation, **3**) or resonance of two or more classical structures. From the stereochemical point of view, those structures are assigned to the nonclassical type for which all tetracoordinate carbon bonds extend into a single hemisphere, i.e., the valence angle of a carbon atom is greater than 180°. A hypothetical example is pyramidane, **4**, the structure of which corresponds to a local minimum on the C_5H_4 potential energy surface.



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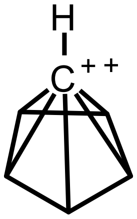

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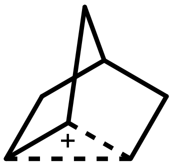

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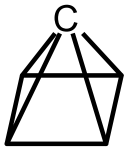

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Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1955

nonselectively labelled

An isotopically labelled compound is designated as nonselectively labelled when the position(s) and the number of the labelling nuclide(s) are both undefined.

Source:
Blue Book, p. 517
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1896

nor-

Affix used to denote the elimination of one methylene group from a side chain of a parent structure (including a methyl group).

Source:
Blue Book, p. 497

normal

The term 'normal' in e.g. 'normal boiling temperature' means the value at a pressure of $101325\ \mathrm{Pa}$.

Source:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 537

normal distribution

See: Gaussian band shape

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2203

normal kinetic isotope effect

See: isotope effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1145

normal region (for electron transfer)

Region for which the rate constants increase with increasing exergonicity of the reaction in plots relating rate constants for electron transfer, or quantities related to it, with the standard Gibbs energy for the reaction ($\Delta_{\mathrm{ET}}G^{\mathrm{o}}$). This region is predicted by the Marcus theory for outer-sphere electron transfer for the case of $-\Delta_{\mathrm{ET}}G^{\mathrm{o}} \leq \lambda$ in the Marcus equation.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 375

normal stress, σ

Force acting normally to a surface divided by the area of the surface.

Source:
Green Book, 2nd ed., p. 12

normal X-ray level

Synonymous with diagram level.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 738

normal-phase chromatography

An elution procedure in which the stationary phase is more polar then the mobile phase. This term is used in liquid chromatography to emphasize the contrast to reversed-phase chromatography.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 826

normalization

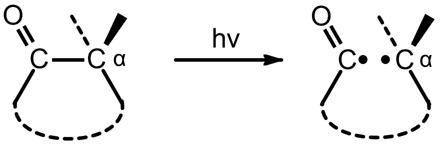
A mathematical procedure which ensures that the integral of the square of modulus of a wave-function over all space equals 1. The constant required to ensure that a wave-function is normalized is termed the normalization constant.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1956

Norrish Type I photoreaction

α-Cleavage of an excited carbonyl compound leading to an acyl-alkyl radical pair (from an acyclic carbonyl compound) or an acyl-alkyl diradical (from a cyclic carbonyl compound) as a primary photoproduct.
Notes:

1. An example is:

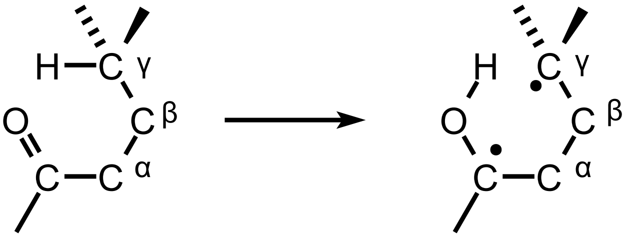


2. Decarbonylation of the primary diradical formed from cyclic carbonyl compounds and subsequent recombination of the biradical afford very interesting cyclic compounds.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 375

Norrish Type II photoreaction

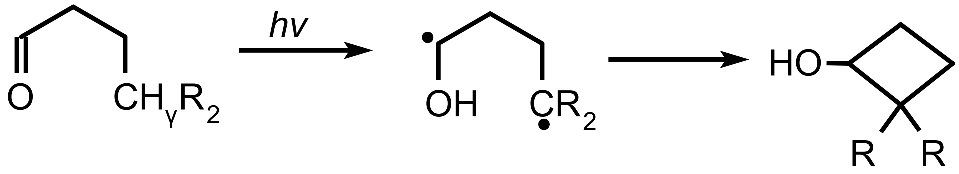
Intramolecular abstraction of a γ-hydrogen by an excited carbonyl compound to produce a 1,4-diradical as a primary photoproduct.
Note:
An example is:



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 375

Norrish–Yang reaction

Photochemical process leading to the formation of cyclobutanols from excited carbonyl compounds by intramolecular γ-hydrogen abstraction (Norrish Type II photoreaction) and subsequent 1,4-diradical combination.



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 375

*n*th order phase transition

A transition in which the molar Gibbs energy (or chemical potential) and its $(n-1)$th-order derivatives are continuous, whereas the nth-order derivatives with respect to temperature and pressure are discontinuous at the transition point.
See: first-order transition, second-order transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 587

nuclear atom

See: coordination entity

Source:
Red Book, p. 145
Blue Book, p. 337

nuclear chemistry

The part of chemistry which deals with the study of nuclei and nuclear reactions using chemical methods.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

nuclear decay

A spontaneous nuclear transformation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518

nuclear disintegration

Nuclear decay involving a splitting into more nuclei or the emission of particles.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1540

nuclear fission

The division of a nucleus into two or more parts with masses of equal order of magnitude, usually accompanied by the emission of neutrons, gamma radiation and, rarely, small charged nuclear fragments.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2519

nuclear fuel

Material containing fissile nuclides, which when placed in a reactor, enables a chain reaction to be achieved.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

nuclear fusion

See: nuclear fusion reaction

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

nuclear fusion reaction

A reaction between two light nuclei resulting in the production of a nuclear species heavier than either initial nucleus.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1543

nuclear graphite

A polygranular graphite material for use in nuclear reactor cores consisting of graphitic carbon of very high chemical purity. High purity is needed to avoid absorption of low-energy neutrons and the production of undesirable radioactive species.
Note:
Apart from the absence of neutron-absorbing impurities, modern reactor graphites are also characterized by a high degree of graphitization and no preferred bulk orientation. Such properties increase the dimensional stability of the nuclear graphite at high temperatures and in a high flux of neutrons. The term nuclear graphite is often, but incorrectly, used for any graphite material in a nuclear reactor, even if it serves only for structural purposes.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 498

nuclear isomers

Nuclides having the same mass number and atomic number, occupying different nuclear energy states.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1545

nuclear level

One of the energy values at which a nucleus can exist for an appreciable time ($> 10^{-22}$ s).

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

nuclear magneton

Electromagnetic fundamental physical constant $\mu_{\mathrm{N}} = \frac{m_{\mathrm{e}}}{m_{\mathrm{p}}} \mu_{\mathrm{B}} = 5.050\ 7866(17) \times 10^{-27}\ \mathrm{J\ T^{-1}}$, where m_{e} is the electron rest mass, m_{p} the proton rest mass and μ_{B} the Bohr magneton.

Source:
CODATA Bull. 1986, *63*, 1

nuclear particle

A nucleus or any of its constituents in any of their energy states.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

nuclear quadrupole moment (spectroscopic)

A parameter which describes the effective shape of the equivalent ellipsoid of the nuclear charge distribution, $Q > 0$ for prolate (e.g. ^{57}Fe, ^{197}Au); $Q < 0$ for oblate (e.g. ^{119}Sn, ^{129}I) nuclei.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 214

nuclear reactor

A device in which a self-sustaining nuclear fission chain reaction can be maintained and controlled. The term is sometimes applied to a device in which a nuclear fusion reaction can be produced and controlled.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

nuclear transformation

The change of one nuclide into another with a different proton number or nucleon number.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1553

nuclear transition

For a nucleus a change from one quantized energy state into another or a nuclear transformation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1553

nuclearity

The number of central atoms joined in a single coordination entity by bridging ligands or metal-metal bonds is indicated by dinuclear, trinuclear, tetranuclear, polynuclear, etc.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1288

nucleating agent

A material either added to or present in a system, which induces either homogeneous or heterogeneous nucleation.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

nucleation and growth

A process in a phase transition in which nuclei of a new phase are first formed, followed by the propagation of the new phase at a faster rate.
See: continuous precipitation, discontinuous precipitation

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 587

nucleation

Also contains definition of: simultaneous nucleation

in colloid chemistry

The process by which nuclei are formed in solution. The condensation of a single chemical compound is called homogeneous nucleation. The simultaneous condensation of more than one compound is called simultaneous nucleation. The condensation of a compound on a foreign substance is called heterogeneous nucleation.

Source:
Orange Book, p. 84

See also:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

nucleation of phase separation

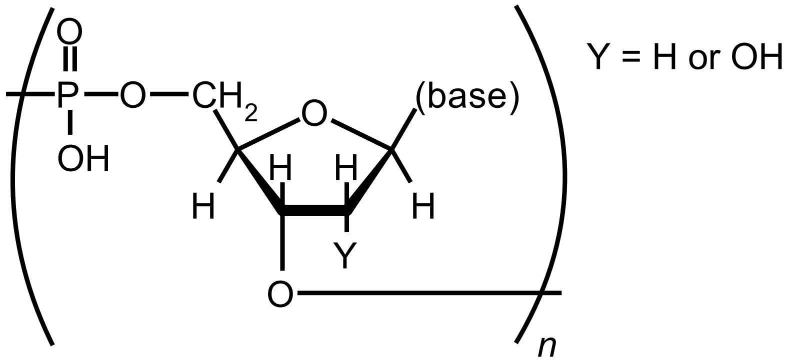
in polymer chemistry

Initiation of phase domain formation through the presence of heterogeneities.
Note:
In a metastable region of a phase diagram, phase separation is initiated only by nucleation.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1997

nucleic acids

Macromolecules, the major organic matter of the nuclei of biological cells, made up of nucleotide units, and hydrolysable into certain pyrimidine or purine bases (usually adenine, cytosine, guanine, thymine, uracil), D-ribose or 2-deoxy-D-ribose and phosphoric acid.



See: ribonucleic acids, , deoxyribonucleic acids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

See also:
White Book, p. 110
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 161

nucleofuge

A leaving group that carries away the bonding electron pair. For example, in the hydrolysis of an alkyl chloride, Cl^- is the nucleofuge. The tendency of atoms or groups to depart with the bonding electron pair is called nucleofugality. The adjective is nucleofugal.
See also: electrofuge, nucleophile

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1145

nucleon

Heavy nuclear particle: proton or neutron.

Source:
Physical Chemistry Division, unpublished

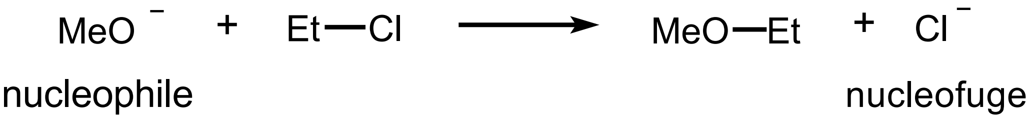
nucleon number

Synonymous with mass number.

Source:
Green Book, 2nd ed., p. 20

nucleophile (nucleophilic)

A nucleophile (or nucleophilic reagent) is a reagent that forms a bond to its reaction partner (the electrophile) by donating both bonding electrons. A 'nucleophilic substitution reaction' is a heterolytic reaction in which the reagent supplying the entering group acts as a nucleophile. For example:



$$\underset{\text{nucleophile}}{\mathrm{MeO^-}} + \mathrm{Et{-}Cl} \longrightarrow \mathrm{MeO{-}Et} + \underset{\text{nucleofuge}}{\mathrm{Cl^-}}$$

The term 'nucleophilic' is also used to designate the apparent polar character of certain radicals, as inferred from their higher relative reactivity with reaction sites of lower electron density. Nucleophilic reagents are Lewis bases.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1146

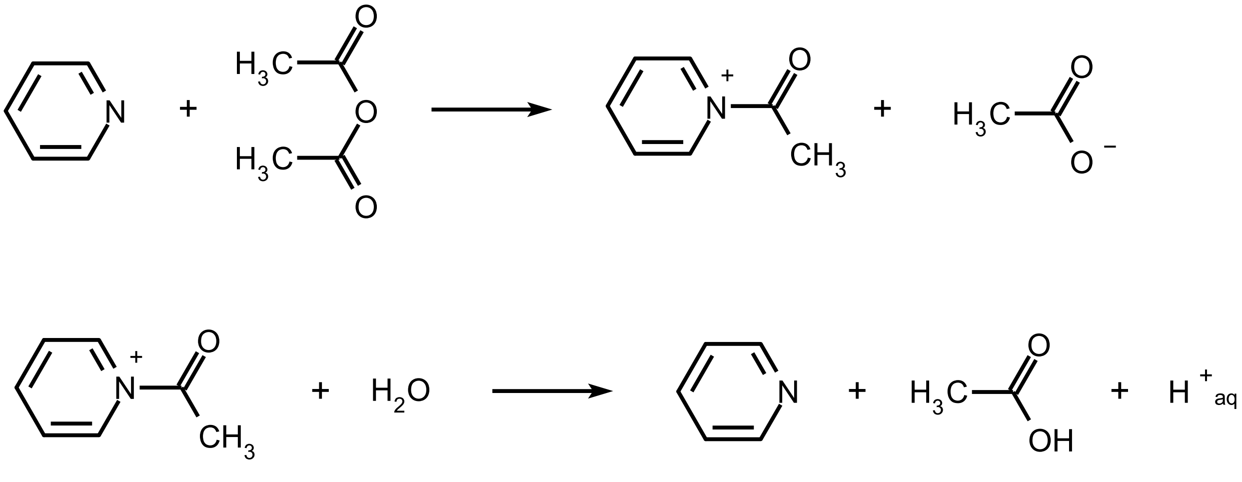
nucleophilic aromatic photosubstitution

Photosubstitution in aromatic compounds with the participation of nucleophiles.
Note:
While electrophilic substitution is the most common reaction on aromatic compounds in the ground state, nucleophilic substitution is typical for the excited states of these compounds. Some electrophilic aromatic photosubstitutions (upon excitation of the aromatic substrate) have been reported.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 376

nucleophilic catalysis

Catalysis by a Lewis base, involving formation of a Lewis adduct as a reaction intermediate. For example, the hydrolysis of acetic anhydride in aqueous solution catalysed by pyridine:

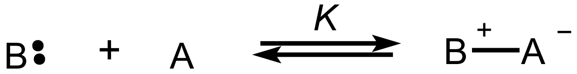


See also: electrophilic, nucleophilicity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1146

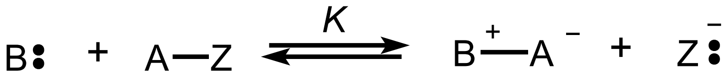
nucleophilicity

1. The property of being nucleophilic.
2. The relative reactivity of a nucleophilic reagent. (It is also sometimes referred to as 'nucleophilic power'.) Qualitatively, the concept is related to Lewis basicity. However, whereas Lewis basicity is measured by relative equilibrium constants:



$$\mathrm{B}\!: + \mathrm{A} \xrightleftharpoons{K} \overset{+}{\mathrm{B}}\!-\!\overset{-}{\mathrm{A}}$$

nucleophilicity of a Lewis base is measured by relative rate constants of different nucleophilic reagents towards a common substrate, most commonly involving formation of a bond to carbon:



$$\mathrm{B}\!: + \mathrm{A{-}Z} \xrightleftharpoons{K} \overset{+}{\mathrm{B}}\!-\!\overset{-}{\mathrm{A}} + \overset{-}{\mathrm{Z}}\!:$$

See also: electrophilicity, Ritchie equation, Swain–Scott equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1146

nucleoproteins

Proteins having nucleic acids as prosthetic groups, and thus yielding nucleic acids (or their cleavage products) as well as amino acids on hydrolytic cleavage.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

nucleosides

Ribosyl or deoxyribosyl derivatives (rarely, other glycosyl derivatives) of certain pyrimidine or purine bases. They are thus glycosylamines or N-glycosides related to nucleotides by the lack of phosphorylation. It has also become customary to include among nucleosides analogous substances in which the glycosyl group is attached to carbon rather than nitrogen ('C-nucleosides').
See also: nucleic acids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

See also:
White Book, p. 110

PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 161

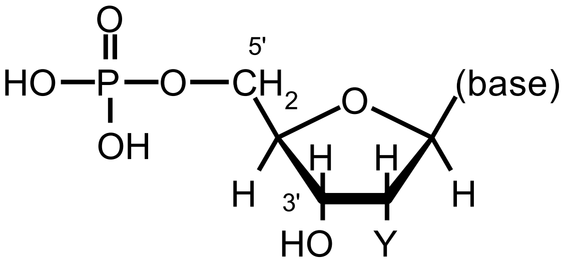
nucleotide bases

The heterocyclic pyrimidine and purine compounds which are constituents of all nucleic acids. Adenine (A), guanine (G) and cytosine (C) are found in both DNA and RNA, thymine (T) is found (primarily) in DNA and uracil (U) only in RNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 147

nucleotides

Compounds formally obtained by esterification of the 3 or 5 hydroxy group of nucleosides with phosphoric acid. They are the monomers of nucleic acids and are formed from them by hydrolytic cleavage.



Y = H, a deoxyribonucleotide
Y = OH, a ribonucleotide

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1352

See also:
White Book, p. 109
White Book, p. 111
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

nucleus

The positively charged central portion of an atom, excluding the orbital electrons.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

nuclide

A species of atom, characterized by its mass number, atomic number and nuclear energy state, provided that the mean life in that state is long enough to be observable.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522
Red Book, p. 35
Orange Book, p. 233
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

nuclidic mass

The rest mass of a nuclide expressed in atomic mass units.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

nuisance threshold

in atmospheric chemistry

That concentration of an air pollutant that is considered objectionable. In the case of a substance with an objectionable odour, it is the smallest concentration of the substance which can be detected by a human being (nose).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2203

number concentration, C, n

Number of entities of a constituent in a mixture divided by the volume of the mixture.
See: concentration

Source:
Green Book, 2nd ed., p. 39
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 984

number content, $\frac{N_B}{m}$

Number of defined particles, or elementary entities, of a component in a system divided by the mass of that system.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 984

number density, n

Number of particles divided by the volume they occupy.

Source:
Green Book, 2nd ed., p. 39
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2183

number flow rate, q_N

Number of defined particles, or elementary entities of a defined component, crossing a cross-section divided by the time.
See: mass flow rate, volume flow rate

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 984

number fraction

See: amount fraction

Source:
Green Book, 2nd ed., p. 41
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 984

number of entities, N

Integer number obtained by counting of entities, which are usually molecules atoms or ions.

Source:
Green Book, 2nd ed., p. 39
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 985

number-distribution function

A distribution function in which the relative amount of a portion of a substance with a specific value, or a range of values, of the random variable(s) is expressed in terms of mole fraction.

Source:
Purple Book, p. 56

numerical value

of a quantity

Quotient of the value of a quantity and the unit used in its expression.
See: value *of a quantity*

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 985

observation height, h_{obs}

in flame emission and absorption spectrometry

The difference in height between the axis of the observed space (optical axis) and the burner tip (in mm). The optical axis of the instrument should be the same as the optical axis of the observation space. Other definitions which express the observation height as a fraction of the whole flame height are not recommended because the height to the tip of the flame is not well defined. The observation height should be stated in the method.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1741

observation pathlength, l_{obs}

in flame emission and absorption spectrometry

The intersection of the optical axis and the observation space (in mm).

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1741

observation space

in flame emission and absorption spectrometry

The intersection of the optical beam and that part of the flame where the net signal is at least half of the maximum net signal. The characteristics of the observation space depend on the temperature of the flame, the stoichiometry of the gases and the properties of the processed fluid (presence of proteins for instance). The observation space in atomic absorption is analogous to the observation space of a cuvette in molecular absorption spectrometry.
See also: observation volume

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1741

observation volume, V_{obs}

in flame emission and absorption spectrometry

The volume of that part of the flame that is observed through the optical device (in μl).
See also: observation space

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1741

occlusion (molecular)

The process of incorporation of foreign substances as molecular species within precipitates as they are formed.

Source:
Orange Book, p. 85

octahedro-

in inorganic nomenclature

An affix used in names to denote six atoms bound into an octahedron.

Source:
Red Book, p. 245
Blue Book, p. 465

odd-electron ion

Synonymous with radical ion.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

ODMR (Optically Detected Magnetic Resonance)

Also contains definitions of: ADMR, DEDMR, DFDMR, PDMR, RYDMR

A double resonance technique in which transitions between spin sublevels are detected by optical means. Usually these are sublevels of a triplet and the transitions are induced by microwaves. For different types of optical detection the following expressions are used: ADMR (absorption), DEDMR (delayed emission, non-specified), DFDMR (delayed fluorescence), FDMR (fluorescence), PDMR (phosphorescence). If a reaction yield is followed the expression RYDMR (reaction yield detected magnetic resonance) is used.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2257

odour threshold

in atmospheric chemistry

The concentration of a compound which produces an odour which is detectable by a human being (nose). For certain compounds this threshold is very low (e.g. 1 part in 10^9 for certain sulfides).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2204

ohm

SI derived unit of electrical resistance, $\Omega = \mathrm{V\ A^{-1}} = \mathrm{m^2\ kg\ s^{-3}\ A^{-2}}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 985

OLED

Acronym for <u>o</u>rganic <u>l</u>ight-<u>e</u>mitting <u>d</u>evice.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 377

olefins

Acyclic and cyclic hydrocarbons having one or more carbon–carbon double bonds, apart from the formal ones in aromatic compounds. The class olefins subsumes alkenes and cycloalkenes and the corresponding polyenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1353

oligo

A prefix meaning 'a few', and used for compounds with a number of repeating units intermediate between those in monomers and those in high polymers. The limits are not precisely defined, and in practice vary with the type of structure being considered, but are generally from 3 to 10, e.g. oligopeptides, oligosaccharides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1353

oligomer

Also contains definition of: telomer

A substance composed of oligomer molecules. An oligomer obtained by telomerization is often termed a telomer.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2289

oligomer molecule

Also contains definition of: oligomeric

A molecule of intermediate relative molecular mass, the structure of which essentially comprises a small plurality of units derived, actually or conceptually, from molecules of lower relative molecular mass.

Notes:

1. A molecule is regarded as having an intermediate relative molecular mass if it has properties which do vary significantly with the removal of one or a few of the units.
2. If a part or the whole of the molecule has an intermediate relative molecular mass and essentially comprises a small plurality of units derived, actually or conceptually, from molecules of lower relative molecular mass, it may be described as oligomeric, or by oligomer used adjectivally.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2289

oligomerization

The process of converting a monomer or a mixture of monomers into an oligomer. An oligomerization by chain reaction carried out in the presence of a large amount of chain-transfer agent, so that the end-groups are essentially fragments of the chain transfer agent, is termed telomerization.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2306

oligonucleotides

See: oligo, nucleotides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1353

See also:
White Book, p. 111

oligopeptides

See: oligo, peptides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1353

See also:
White Book, p. 48

oligosaccharides

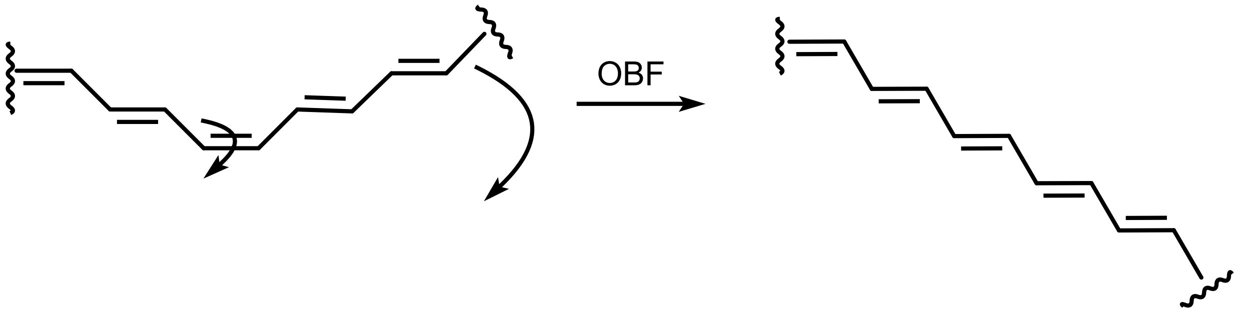
See: oligo, saccharides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1353

one-bond-flip

Acronym: OBF

Photoisomerization of one double bond in a conjugated double bond system. It is a regular *E/Z* photoisomerization.



Compare with bicycle-pedal mechanism, hula-twist mechanism.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 377

one-photon photochromism

Photochromic process involving a one-photon mechanism. In this case, the photoproduct B is formed from the singlet or from the triplet state of the thermodynamically-stable molecular entity A.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 377

onion morphology

Multiphase morphology of roughly spherical shape that comprises alternating layers of different polymers arranged concentrically, all layers being of similar thickness.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2004

onium compounds

1. Cations (with their counter-ions) derived by addition of a hydron to a mononuclear parent hydride of the nitrogen, chalcogen and halogen families.
   (H_4N^+) ammonium
   (H_3O^+) oxonium
   (H_2F^+) fluoronium
   (H_4P^+) phosphonium
   (H_3S^+) sulfonium
   (H_2Cl^+) chloronium
   (H_4As^+) arsonium
   (H_3Se^+) selenonium
   (H_2Br^+) bromonium
   (H_4Sb^+) stibonium
   (H_3Te^+) telluronium
   (H_2I^+) iodonium
   (H_4Bi^+) bismuthonium
2. Derivatives formed by substitution of the above parent ions by univalent groups. The number of substituted hydrogen atoms is, especially in the case of hydrocarbyl substituents, indicated by the adjectives primary, secondary, tertiary or quaternary. E.g. (Cl_2F^+) dichlorofluoronium, $(CH_3)_2S^+H$ dimethylsulfonium (a secondary sulfonium ion), $Cl(CH_3)_3P^+$ chlorotrimethylphosphonium, $(CH_3CH_2)_4N^+$ tetraethylammonium (a quaternary ammonium ion).
   See also: arsonium compounds, halonium ions, oxonium ions, phosphonium compounds, quaternary ammonium compounds, stibonium compounds, sulfonium compounds
3. Derivatives formed by substitution of the above parent ions by groups having two or three free valencies on the same atom. Such derivatives are, where possible, designated by a specific class name. E.g. $RC{\equiv}O^+$ hydrocarbylidyne oxonium ions, $R_2C{=}N^+H_2X^-$ iminium compounds, $RC{\equiv}NH^+$ nitrilium ions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1353

PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1146

open film

Also contains definitions of: closed film, partly open film

A film in which mass transfer can occur between the film and the coexisting bulk phases, for all the components. The term partly open film applies to a film in which mass transfer can occur only for certain components. The term closed film applies to those films with fixed mass.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1671

open hearth furnace

in atmospheric chemistry

Reverberatory furnace, containing a basin-shaped hearth, for melting and refining suitable types of pig iron, iron ore, and scrap for steel production. A large amount of dust from ore and other materials and splashings from slag are carried away by the waste gases; a supplementary chamber is commonly used for collecting slag and dust.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2204

open-shell systems

Atomic or molecular systems in which the electrons are not completely assigned to orbitals in pairs.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1956

open-tubular column

in chromatography

A column, usually having a small diameter, in which either the inner tube wall, or a liquid or active solid held stationary on the tube wall acts as the stationary phase and there is an open, unrestricted path for the mobile phase.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831
Orange Book, p. 97

operational pH cell

An electrochemical cell which is the basis of practical pH measurement consisting of a hydrogen ion-responsive electrode (hydrogen gas, or glass) and a reference electrode immersed in the test solution.
See: pH

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 540

operational pH standard

Certain substances which meet the criteria of (i) preparation in highly pure state reproducibly and (ii) stability of solution over a reasonable period of time are designated as operational standards in aqueous solution of specified concentration. Their number is in principle unlimited but values are available now for 15 solutions. The values of operational pH standard, i.e. $\mathrm{pH(OS)}$, are assigned by comparison with the reference value pH standard, i.e. $\mathrm{pH(RVS)}$, in cells with liquid junction, the operational cells, where the liquid junctions are formed within vertical $1\ \mathrm{mm}$ tubes.

$$\mathrm{Pt}\ |\ \mathrm{H_2}\ |\ \mathrm{OS}\ \|\ \underset{> 3.5\ \mathrm{mol\ dm^{-3}}}{\mathrm{KCl}}\ \|\ \mathrm{RVS}\ |\ \mathrm{H_2}\ |\ \mathrm{Pt\ (Pd)}$$

Source:
Orange Book, p. 21

operator gene

See: operon

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

operon

A functional unit consisting of a promoter, an operator and a number of structural genes, found mainly in prokaryotes. The structural genes commonly code for several functionally related enzymes, and although they are transcribed as one (polycistronic) mRNA each is independently translated. In the typical operon, the operator region acts as a controlling element in switching on or off the synthesis of mRNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

opposing reactions

Composite reactions, occurring in forward and reverse directions:

$$\mathrm{A} + \mathrm{B} \underset{-1}{\overset{1}{\rightleftharpoons}} \mathrm{Z}$$

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2296
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1146

optical activity

A sample of material able to rotate the plane of polarization of a beam of transmitted plane-polarized light is said to possess optical activity (or to be optically active). This optical rotation is the classical distinguishing characteristic (sufficient but not necessary) of systems containing unequal amounts of corresponding enantiomers. An enantiomer causing rotation in a clockwise direction (when viewed in the direction facing the oncoming light beam) under specified conditions is called dextrorotatory and its chemical name or formula is designated by the prefix (+)-; one causing rotation in the opposite sense is laevorotatory and designated by the prefix (−)-. Materials with optical activity also exhibit other chiroptic phenomena.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

optical antipodes [obsolete]

Obsolete synonym for enantiomers. (Usage strongly discouraged).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

optical density [obsolete]

Synonymous with absorbance. The use of the term optical density is discouraged.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2257

optical filter

Also contains definition of: interference filter

A device which reduces the spectral range (bandpass, cut-off, and interference filter) or radiant power of incident radiation (neutral density or attenuance filter) upon transmission of radiation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2257

optical isomers **[obsolete]**

Obsolescent synonym for stereoisomers with different optical properties. They should be described as diastereoisomers or enantiomers. (Usage strongly discouraged).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

optical multi-channel analyser

Acronym: OMA

Detection system for fast acquisition of spectra. It consists of a 'polychromator' fitted with a detector that enables spatial resolution, e.g., a 'vidicon tube', a 'charge-coupled device' or a 'silicon photodiode array'.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 378

optical parametric amplification

Acronym: OPA

Process of signal amplification by a parametric process and a pump wave.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 378

optical parametric oscillator

Acronym: OPO

Light source similar to a laser, but based on 'non-linear optical gain' from parametric amplification rather than on stimulated emission.
Notes:

1. The device is a powerful solid-state source of broadly tunable coherent radiation. It consists of a crystal, usually BBO (BaB_2O_4), located inside an optical resonator and pumped by a very intense laser beam (typically provided by a pulsed neodymium laser or a diode laser). The pump beam (wavelength λ_p frequency ν_p) is partially converted into two coherent beams, the signal and the idler, with wavelengths (λ_s, λ_I) and frequencies (ν_s, ν_I) such that $\nu_s + \nu_i = \nu_p$. By simultaneous rotation of the crystal and adjustment of the optical resonator, the wavelength of the signal beam is continuously tunable, theoretically from λ_p to $2 \times \lambda_p$ and practically over a slightly more reduced range.
2. For example, for $\lambda_p = 355\ \mathrm{nm}$ (3^{rd} harmonic of a Nd:YAG laser), ν_s can be tuned from $400\ \mathrm{nm}$ (with $\lambda_i \approx 3.15\ \mu\mathrm{m}$) up to $600\ \mathrm{nm}$ (with $\lambda_i \approx 870\ \mathrm{nm}$).
3. This 'splitting of one photon into two photons' is the reverse of the 'sum frequency mixing' used, for instance, to generate the 3^{rd} harmonic of a laser emission by mixing in a convenient crystal the fundamental and the frequency doubled beams (a way to get the 3^{rd} harmonic much more efficiently than by pure frequency tripling as described under harmonic frequency generation).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 378

optical purity

The ratio of the observed optical rotation of a sample consisting of a mixture of enantiomers to the optical rotation of one pure enantiomer.
See: enantiomeric excess

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

optical resolution [obsolete]

Usage strongly discouraged.
See: resolution

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

optical rotation

See: optical activity

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

optical rotatory power

Angle of optical rotation divided by the optical path length through the medium and by either the mass concentration of the substance giving the specific optical rotatory power $[\alpha]_{\lambda}^{\theta}$ or by amount concentration, giving the molar optical rotatory power, α_{m}.

Source:
Green Book, 2nd ed., p. 33

optical spectroscopy

The study of systems by the electromagnetic radiation with which they interact or that they produce. By convention, spectroscopic properties are expressed in terms of wavelength *in vacuo*, not the wavelength within the medium being studied.

Source:
PAC, 1985, *57*, 105 *(Names, symbols, definitions and units of quantities in optical spectroscopy (Recommendations 1984))* on page 107

optical yield

In a chemical reaction involving chiral reactants and products, the ratio of the optical purity of the product to that of the precursor, reactant or catalyst. This should not be confused with enantiomeric excess. The optical yield is in no way related to the chemical yield of the reaction.
See: stereoselectivity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1146
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

optical-beam error

in spectrochemical analysis

For wavelength-scanning spectrometers, an error may be introduced if the image position on the photodetector changes. Reflection of the incident radiation, e.g. between the cell walls, is another source of error and results in a measured absorbance slightly higher than the true absorbance. These errors are collectively termed optical-beam errors.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1457

optically active polymer

Polymer capable of rotating the polarization plane of a transmitted beam of linear-polarized light.
Notes:

1. ***See also:*** optical activity.
2. The optical activity originates from the presence of chiral elements in a polymer such as chiral centers or chiral axes due to long-range conformational order in a polymer (helicity) (***See also:*** helicity).

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 900

optically labile [obsolete]

A term describing a system in which stereoisomerization results in a change of optical rotation with time. (Usage strongly discouraged).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

optoacoustic spectroscopy

Same as photoacoustic spectroscopy.
Note:
Frequently used to denominate the laser-induced production of acoustic waves combined with a piezoelectric detector and distinguish it from the amplitude-modulated excitation combined with a gas-coupled microphone as detector.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 379

orbital (atomic or molecular)

Wavefunction depending explicitly on the spatial coordinates of only one electron.
See also: atomic orbital, molecular orbital

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 379

orbital energy

Eigenvalue of a one-electron effective hamiltonian belonging to an orbital.

Source:
Green Book, 2nd ed., p. 18

orbital steering

A concept expressing that the stereochemistry of approach of two reacting species is governed by the most favourable overlap of their appropriate orbitals

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1147

orbital symmetry

The behaviour of an atomic or localized molecular orbital under molecular symmetry operations characterizes its orbital symmetry. For example, under a reflection in an appropriate symmetry plane, the phase of the orbital may be unchanged (symmetric), or it may change sign (antisymmetric), i.e. the positive and negative lobes are interchanged. A principal context for the use of orbital symmetry is the discussion of chemical changes that involve 'conservation of orbital symmetry'. If a certain symmetry element (e.g. the reflection plane) is retained along a reaction pathway, that pathway is 'allowed' by orbital symmetry conservation if each of the occupied orbitals of the reactant(s) is of the same symmetry type as a similarly (e.g. singly or doubly) occupied orbital of the product(s). This principle permits the qualitative construction of correlation diagrams to show how molecular orbitals transform (and how their energies change) during idealized chemical changes (e.g. cycloadditions). An idealized single bond is a σ-bond, i.e. it has cylindrical symmetry, whereas a p-orbital or π-bond orbital has π-symmetry, i.e. it is antisymmetric with respect to reflection in a plane passing through the atomic centres with which it is associated. In ethene, the π-bonding orbital is symmetric with respect to reflection in a plane perpendicular to and bisecting the C–C bond, whereas the π*-antibonding orbital is antisymmetric with respect to this operation. Considerations of orbital symmetry are frequently grossly simplified in that, for example, the p-orbitals of a carbonyl group would be treated as having the same symmetry as those of ethene, and the fact that the carbonyl group in, for example, camphor, unlike that in formaldehyde, has no mirror planes would be ignored. These simplified considerations nevertheless afford the basis of one approach to the understanding of the rules which indicate whether pericyclic reactions are likely to occur under thermal or photochemical conditions.
See also: sigma, pi

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1147

order of reaction, n

Also contains definitions of: observed rate coefficient, partial order of reaction, pseudo-first-order rate coefficient, rate constant, k

If the macroscopic (observed, empirical or phenomenological) rate of reaction (v) for any reaction can be expressed by an empirical differential rate equation (or rate law) which contains a factor of the form $k\,[\mathrm{A}]^{\alpha}\,[\mathrm{B}]^{\beta}$ ... (expressing in full the dependence of the rate of reaction on the concentrations $[\mathrm{A}]$, $[\mathrm{B}]$ ...) where α, β are constant exponents (independent of concentration and time) and k is independent of $[\mathrm{A}]$ and $[\mathrm{B}]$ etc. (rate constant, rate coefficient), then the reaction is said to be of order α with respect to A, of order β with respect to B, ... , and of (total or overall) order

$n = \alpha + \beta + ...$ The exponents α, β, ... can be positive or negative integral or rational nonintegral numbers. They are the reaction orders with respect to A, B, ... and are sometimes called 'partial orders of reaction'. Orders of reaction deduced from the dependence of initial rates of reaction on concentration are called 'orders of reaction with respect to concentration'; orders of reaction deduced from the dependence of the rate of reaction on time of reaction are called 'orders of reaction with respect to time'. The concept of order of reaction is also applicable to chemical rate processes occurring in systems for which concentration changes (and hence the rate of reaction) are not themselves measurable, provided it is possible to measure a chemical flux. For example, if there is a dynamic equilibrium according to the equation:

$$a\,\mathrm{A} \rightleftharpoons p\,\mathrm{P}$$

and if a chemical flux is experimentally found, (e.g. by NMR line-shape analysis) to be related to concentrations by the equation:

$$\frac{\varphi_{-\mathrm{A}}}{\alpha} = k\,[\mathrm{A}]^{\alpha}\,[\mathrm{L}]^{\lambda}$$

then the corresponding reaction is of order α with respect to A ... and of total (or overall) order $n(= \alpha + \lambda + ...)$. The proportionality factor k above is called the (nth order) 'rate coefficient'. Rate coefficients referring to (or believed to refer to) elementary reactions are called 'rate constants' or, more appropriately 'microscopic' (hypothetical, mechanistic) rate constants. The (overall) order of a reaction cannot be deduced from measurements of a 'rate of appearance' or 'rate of disappearance' at a single value of the concentration of a species whose concentration is constant (or effectively constant) during the course of the reaction. If the overall rate of reaction is, for example, given by:

$$v = k\,[\mathrm{A}]^{\alpha}\,[\mathrm{B}]^{\beta}$$

but [B] stays constant, then the order of the reaction (with respect to time), as observed from the concentration change of A with time, will be α, and the rate of disappearance of A can be expressed in the form:

$$v_{\mathrm{A}} = k_{\mathrm{obs}}\,[\mathrm{A}]^{\alpha}$$

The proportionality factor k_{obs} deduced from such an experiment is called the 'observed rate coefficient' and it is related to the $(\alpha + \beta)$th order rate coefficient k by the equation:

$$k_{\mathrm{obs}} = k\,[\mathrm{B}]^{\beta}$$

For the common case when $\alpha = 1$, k_{obs} is often referred to as a 'pseudo-first order rate coefficient' (k_{ψ}). For a simple (elementary) reactions a partial order of reaction is the same as the stoichiometric number of the reactant concerned and must therefore be a positive integer (see rate of reaction). The overall order is then the same as the molecularity . For stepwise reactions there is no general connection between stoichiometric numbers and partial orders. Such reactions may have more complex rate laws, so that an apparent order of reaction may vary with the concentrations of the chemical species involved and with the progress of the reaction: in such cases it is not useful to speak of orders of reaction, although apparent orders of reaction may be deducible from initial rates. In a stepwise reaction, orders of reaction may in principle always be assigned to the elementary steps.

See also: kinetic equivalence

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1147
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2296
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 176
Green Book, 2nd ed., p. 55

order parameter

A normalized parameter that indicates the degree of order of a system. An order parameter of 0 indicates disorder; the absolute value in the ordered state is 1.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 587

order-disorder transition

A transition in which the degree of order of the system changes. Three principal types of disordering transitions may be distinguished: (i) positional disordering in a solid, (ii) orientational disordering which may be static or dynamic and (iii) disordering associated with electronic and nuclear spin states.
Examples:

1. The transition of $LiFeO_2$, with a tetragonal unit cell, in which the Li^+ and Fe^{3+} cations are perfectly ordered on crystallographically non-equivalent octahedral sites to cubic $LiFeO_2$ in which the Li^+ and Fe^{3+} cations are distributed randomly over all the octahedral sites.
2. The transition of orthorhombic KCN to cubic KCN in which the CN^- ions become oriented in any of the eight [111] directions.
3. A superconducting transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 587

ordered co-continuous double gyroid morphology

Co-continuous morphology in which a set of two gyroid-based phase domains exhibits a highly regular, three-dimensional lattice-like morphology with Ia3d space group symmetry.
Notes:

1. The domains are composed of tripoidal units as the fundamental building structures.
2. The two domains are interlaced.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2004

organelles

Separated compartments within a cell with specialized functions, e.g. nuclei (containing most of the genetic material), mitochondria (respiratory energy supply for the cell), chloroplasts (location of photosynthesis) etc.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

organic dye laser

A liquid laser in which the active medium is an organic dye in a solvent.

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1921

organically modified silica

Also contains definition of: organically modified silicate

Silica modified by organic groups.
Notes:

1. Organically-modified silicas can be obtained by sol-gel processing.
2. An organically modified silica is of general structure $(RO)_a Si(B)_b (C)_c (D)_d$, where $(a+b+c+d)=4$, R is any alkyl, aryl or heteroaryl group and B, C and D are generally organic groups.
3. Though it is a commonly used acronym for organically modified silica, 'Ormosil' is a trademark and as such its terminological use is discouraged.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1816

organically-modified ceramic

Also contains definition of: organomodified ceramic

Chemically bonded hybrid material which is a crosslinked inorganic–organic polymer.
Notes:

1. Organically modified ceramics are hybrid polymers with inorganic and organic moieties linked by stable covalent bonds and based on organically modified alkoxysilanes, functionalized organic polymers or both.
2. Though it is a commonly used acronym for organically modified ceramic, 'Ormocer' is a registered trademark and as such its terminological use is strongly discouraged.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1816

organic–inorganic polymer

Acronym: OIP

Polymer or polymer network with aff skeletal structure comprised only of carbon but which has side-groups that include inorganic components.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1816

organo-

See: organometallic compounds, organoheteryl groups

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1353

organoheteryl groups

Univalent groups containing carbon, which are thus organic, but which have their free valence at an atom other than carbon. This collective term is seldom used; specific subclasses are more frequently encountered (organothio or organylthio, organogermanium or organylgermanium groups). The synonymous term organoelement groups is occasionally encountered. E.g. phenoxy, acetamido, pyridinio ($C_5H_5N^+$), thiocyanato ($N{\equiv}C{-}S^-$), trimethylsilyl; but not hydroxyphenyl, aminoacetyl.
See: organyl

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1353

organometallic compounds

Classically compounds having bonds between one or more metal atoms and one or more carbon atoms of an organyl group. Organometallic compounds are classified by prefixing the metal with organo-, e.g. organopalladium compounds. In addition to the traditional metals and semimetals, elements such as boron, silicon, arsenic and selenium are considered to form organometallic compounds, e.g. organomagnesium compounds MeMgI iodo(methyl)magnesium, Et_2Mg diethylmagnesium; an organolithium compound BuLi butyllithium; an organozinc compound $ClZnCH_2C(=O)OEt$ chloro(ethoxycarbonylmethyl)zinc; an organocuprate $Li^+[CuMe_2]^-$ lithium dimethylcuprate; an organoborane Et_3B triethylborane. The status of compounds in which the canonical anion has a delocalized structure in which the negative charge is shared with an atom more electronegative than

carbon, as in enolates, may vary with the nature of the anionic moiety, the metal ion, and possibly the medium; in the absence of direct structural evidence for a carbon–metal bond, such compounds are not considered to be organometallic.
See: acetylides, ferrocenophanes, Grignard reagents, metallocenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1353

organyl groups

Any organic substituent group, regardless of functional type, having one free valence at a carbon atom, e.g. $CH_3CH_2–$, $ClCH_2–$, $CH_3C(=O)–$, 4-pyridylmethyl. Organyl is also used in conjunction with other terms, as in organylthio- (e.g. MeS–) and organyloxy.
See: heterocyclyl groups, hydrocarbyl, organoheteryl

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

origin of replication (ori)

A sequence of DNA at which replication is initiated on a chromosome, plasmid or virus.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

ortho acids

Hypothetical compounds having the structure $RC(OH)_3$. Thus hydrated forms of carboxylic acids. Orthocarbonic acid, $C(OH)_4$, is generically included.
See also: ortho amides, ortho esters

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

ortho amides

Hypothetical compounds having the structure $RC(NH_2)_3$, and *N*-substituted derivatives thereof. $(R_2N)_4C$ are generically included, but such use is obsolescent.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

ortho esters

Compounds having the structure RC(OR')$_3$ (R' $\neq$ H), or the structure C(OR')$_4$ (R' $\neq$ H), e.g. HC(OCH$_3$)$_3$ trimethyl orthoformate, C(OCH$_3$)$_4$ tetramethyl orthocarbonate.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

ortho- and *peri*-fused (polycyclic compounds)

Polycyclic compounds in which one ring contains two, and only two, atoms in common with each of two or more rings of a contiguous series of rings. Such compounds have *n* common faces and less than 2*n* common atoms. Examples:

7 common faces
8 common atoms

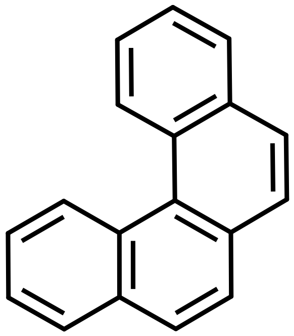
5 common faces
6 common atoms

"*ortho*- and*peri*- fused" systems

Source:
Blue Book, p. 22

ortho-fused (polycyclic compounds)

Polycyclic compounds in which two rings have two, and only two, atoms in common. Such compounds have *n* common faces and 2*n* common atoms. Examples:



3 common faces
6 common atoms

"*ortho*-fused" system

Source:
Blue Book, p. 22

orthokinetic aggregation

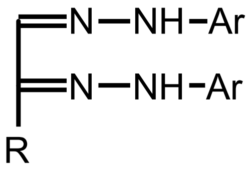
in colloids

The rate of aggregation is in general determined by the frequency of collisions and the probability of cohesion during collision. If the collisions are caused by hydrodynamic motions (e.g convection or sedimentation) this is then referred to as orthokinetic aggregation.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

osazones

1,2-Bis(arylhydrazones) of ketoaldoses (aldoketoses) formed from aldoses and 2-ketoses by reaction with excess arylhydrazine.



R = rest of monosaccharide chain

See: glycosides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

oscillating reaction

A reaction is said to be oscillating if the concentration of one or more intermediates does not vary monotonically, but passes through maximum and minimum values.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 176

oscillator strength, f_{ij}

Measure for integrated intensity of electronic transitions and related to the Einstein transition probability coefficient A_{ij} by:

$$f_{ij} = 1.4992 \times 10^{-14} \frac{A_{ij}}{s^{-1}} \left(\frac{\lambda}{\mathrm{nm}}\right)^2,$$

where λ is the transition wavelength. There are, however, differing uses of f.

Source:
Green Book, 2nd ed., p. 33

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2257

osmolality, m

Quotient of the negative natural logarithm of the rational activity of water and the molar mass of water.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 985

osmotic coefficient, ϕ

Quantity characterizing the deviation of the solvent from ideal behaviour referenced to Raoult's law. The osmotic coefficient on a molality basis is defined by:

$$\phi = \frac{\mu_A^* - \mu_A}{R\,T\,M_A \sum_i m_i}$$

and on an amount fraction basis by:

$$\phi = \frac{\mu_A^* - \mu_A}{R\,T \ln x_A}$$

where μ_A^* and μ_A are the chemical potentials of the solvent as a pure substance and in solution, respectively, M_A is its molar mass, x_A its amount fraction, R the gas constant and T the temperaure. The latter osmotic coefficient is sometimes called the rational osmotic coefficient.

Source:
Green Book, 2nd ed., p. 51
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 546

osmotic concentration, *c*

Synonym: osmolarity

Product of the osmolality and the mass density of water. Formerly called osmolarity.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 985

osmotic pressure, *Π*

Excess pressure required to maintain osmotic equilibrium between a solution and the pure solvent separated by a membrane permeable only to the solvent:

$$\Pi = -\frac{R\,T}{V_A} \ln a_A$$

where V_A, a_A are the partial molar volume and activity of solvent A for an incompressible fluid. For ideal dilute solutions, $\Pi = c_B\,R\,T = \rho_B\,\frac{R\,T}{M_B}$, where entities B are individually moving solute molecules, ions, etc., regardless of their nature, c_B, ρ_B are the amount and mass concentration of the solutes, and M_B is the mass average molar mass of the solutes. The amount is sometimes expressed in osmol (meaning a mole of osmotically active entities), but this usage and the corresponding term osmolarity are discouraged.

Source:
Green Book, 2nd ed., p. 51
Green Book, 3rd ed., p. 59

osones [obsolete]

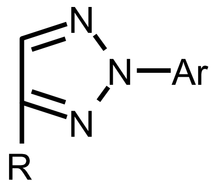
An obsolescent and non-recommended term for 1,2-ketoaldoses, usually derived by hydrolysis of osazones.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

White Book, p. 132

osotriazoles

The 1,2,3-triazoles formed on oxidizing osazones.



R = rest of monosaccharide chain

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

Ostwald ripening

Dissolution of small crystals or sol particles and the redeposition of the dissolved species on the surfaces of larger crystals or sol particles.
Notes:
1. The process occurs because smaller particles have a higher surface energy, hence higher total Gibbs energy, than larger particles, giving rise to an apparent higher solubility.
2. Modified from previous definition. The definition proposed here is recommended for its inclusion of sol particles.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1824

out-isomer

See: in-out isomerism

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2212

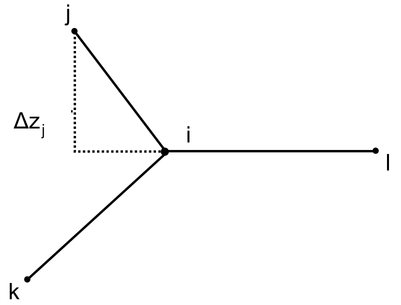
out-of-plane bending coordinate

in molecular geometry

Given by

$$\Delta\theta_{i-jkl} = \frac{\Delta z_j}{r_{eij}} \sin \Phi_{kil}$$

where the numbering of the atoms is given in the diagram. Φ_{kil} denotes



the angle between the bonds ik and il, Δz_j the perpendicular distance of the atom j from the instantaneous plane ikl and r_{eij} the equilibrium length of the bond ij.

Source:
PAC, 1978, *50*, 1707 *(Definition and symbolism of molecular force constants)* on page 1710

outer electric potential, ψ

Electric potential outside the phase concerned. For a conducting sphere of excess charge Q and radius r in vacuum $\psi = \frac{Q}{4\,\pi\,\varepsilon_0\,r}$.

Source:
Green Book, 2nd ed., p. 59

outer Helmholtz plane (OHP)

At an electrified interface, the locus of the electrical centres of non-specifically adsorbed ions in their position of closest approach.

Source:
PAC, 1991, *63*, 895 *(Nomenclature, symbols, definitions and measurements for electrified interfaces in aqueous dispersions of solids (Recommendations 1991))* on page 900

outer-sphere electron transfer

An outer-sphere electron transfer is a reaction in which the electron transfer takes place with no or very weak ($4\ -\ 16\ \mathrm{kJ\ mol^{-1}}$) electronic interaction between the reactants in the transition state. If instead the donor and the acceptor exhibit a strong electronic coupling, the reaction is described as inner-sphere electron transfer. The two terms derive from studies concerning metal complexes and it has been suggested that for organic reactions the term 'nonbonded' and 'bonded' electron transfer should be used.
See also: inner-sphere electron transfer

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1148
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2257

outgassing

of a catalyst

A form of pretreatment in which a catalyst is heated *in vacuo* to remove adsorbed or dissolved gas.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

output rate

The number of results that is produced by an instrument divided by time of operation.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1664

overall activation energy

See: activation energy

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 151

overlap integral, S_{rs}

Integral over space of the type $\int \psi_r^* \psi_s \mathrm{d}\tau$ where ψ_r and ψ_s are different wavefunctions.

Source:
Green Book, 2nd ed., p. 17

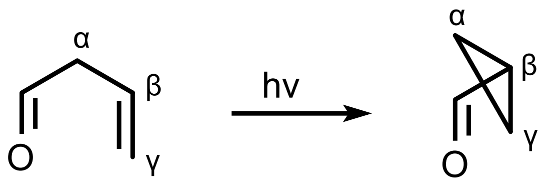
overpotential, η

Deviation of the potential of an electrode from its equilibrium value required to cause a given current to flow through the electrode.

Source:
Green Book, 2nd ed., p. 60

oxa-di-π-methane rearrangement

A photochemical reaction of a β,γ-unsaturated ketone to form a saturated α-cyclopropyl ketone. The rearrangement formally amounts to a 1,2-acyl shift and 'bond formation' between the former α and γ carbon atoms.



See also: di-π-methane rearrangement

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2258

oxenium ions [obsolete]

An unnecessary and erroneous term for oxylium ions, RO^+ ($:\ddot{O}:$ is monooxygen, not 'oxene').

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

oxidant

in atmospheric chemistry

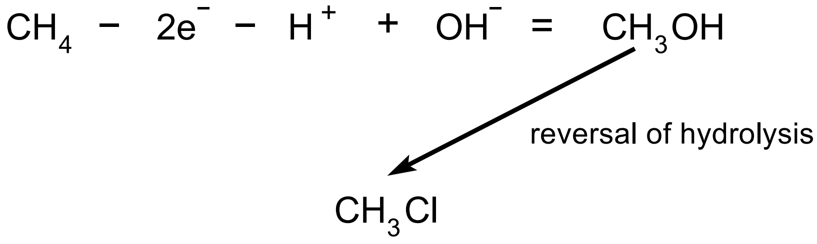
A very qualitative term which includes any and all trace gases which have a greater oxidation potential than oxygen (for example, ozone, peroxyacetyl nitrate, hydrogen peroxide, organic peroxides, NO_3, etc.). It is recommended that alternative, more definitive terms be used which define the specific oxidant of interest whenever possible.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2204

oxidation

1. The complete, net removal of one or more electrons from a molecular entity (also called 'de-electronation').
2. An increase in the oxidation number of any atom within any substrate.
3. Gain of oxygen and/or loss of hydrogen of an organic substrate.

All oxidations meet criteria 1 and 2, and many meet criterion 3, but this is not always easy to demonstrate. Alternatively, an oxidation can be described as a transformation of an organic substrate that can be rationally dissected into steps or primitive changes. The latter consist in removal of one or several electrons from the substrate followed or preceded by gain or loss of water and/or hydrons or hydroxide ions, or by nucleophilic substitution by water or its reverse and/or by an intramolecular molecular rearrangement. This formal definition allows the original idea of oxidation (combination with oxygen), together with its extension to removal of hydrogen, as well as processes closely akin to this type of transformation (and generally regarded in current usage of the term in organic chemistry to be oxidations and to be effected by 'oxidizing agents') to be descriptively related to definition 1. For example the oxidation of methane to chloromethane may be considered as follows:



Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1148

oxidation number

Of a central atom in a coordination entity, the charge it would bear if all the ligands were removed along with the electron pairs that were shared with the central atom. It is represented by a Roman numeral.
Note:
The term Stock number is no longer recommended.

Source:
Red Book, p. 148

See also:
Red Book, p. 66

oxidation state

A measure of the degree of oxidation of an atom in a substance. It is defined as the charge an atom might be imagined to have when electrons are counted according to an agreed-upon set of rules: (l) the oxidation state of a free element (uncombined element) is zero; (2) for a simple (monatomic) ion, the oxidation state is equal to the net charge on the ion; (3) hydrogen has an oxidation state of 1 and oxygen has an oxidation state of -2 when they are present in most compounds. (Exceptions to this are that hydrogen has an oxidation state of -1 in hydrides of active metals, e.g. LiH, and oxygen has an oxidation state of -1 in peroxides, e.g. H_2O_2; (4) the algebraic sum of oxidation states of all atoms in a neutral molecule must be zero, while in ions the algebraic sum of the oxidation states of the constituent atoms must be equal to the charge on the ion. For example, the oxidation states of sulfur in H_2S, S_8 (elementary sulfur), SO_2, SO_3, and H_2SO_4 are, respectively: -2, 0, +4, +6 and +6. The higher the oxidation state of a given atom, the greater is its degree of oxidation; the lower the oxidation state, the greater is its degree of reduction.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2204
NOTE:
Errors in this entry in the printed version of the Compendium (omission of minus signs) have been corrected.

oxidation–reduction (redox) titration

See: titration

Source:
Orange Book, p. 47

oxidative addition

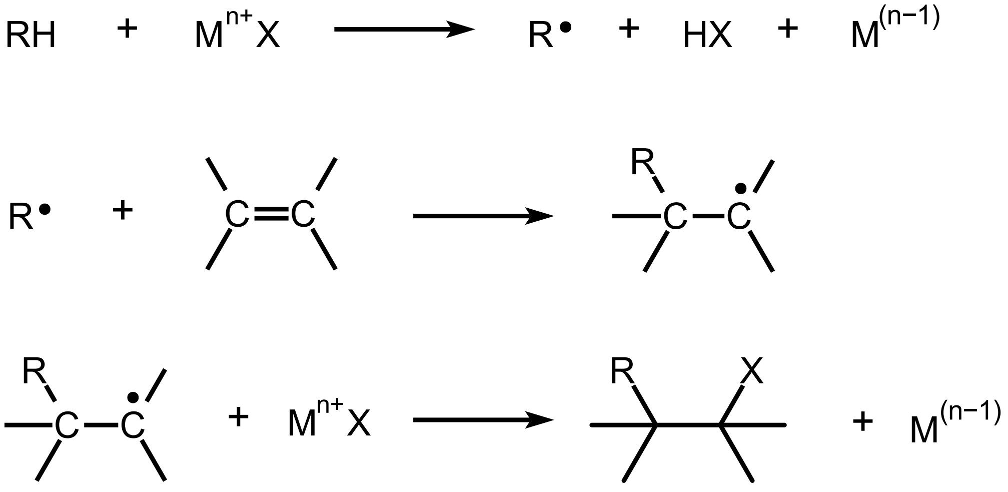
The insertion of a metal complex into a covalent bond involving formally an overall two-electron loss on one metal or a one-electron loss on each of two metals, i.e.

$$\mathrm{L}_n\mathrm{M}^m + \mathrm{XY} \rightarrow \mathrm{L}_n\mathrm{M}^{m+2}(\mathrm{X})(\mathrm{Y}),$$

or

$$2\mathrm{L}_n\mathrm{M}^m + \mathrm{XY} \rightarrow \mathrm{L}_n\mathrm{M}^{m+1}(\mathrm{X}) + \mathrm{L}_n\mathrm{M}^{m+1}(\mathrm{Y})$$

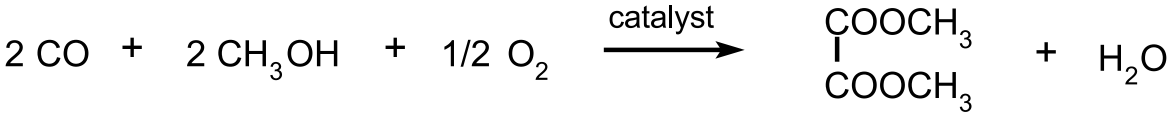
In radical chemistry, the term is used to indicate a radical addition to a carbon–carbon double bond, under oxidative conditions. For example:



Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1149

oxidative coupling

The coupling of two molecular entities through an oxidative process, usually catalysed by a transition metal compound and involving dioxygen as the oxidant; e.g.



$$2\,CO + 2\,CH_3OH + 1/2\,O_2 \xrightarrow{\text{catalyst}} \begin{array}{c} COOCH_3 \\ | \\ COOCH_3 \end{array} + H_2O$$

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1149

oxide network

Network comprising only metal–oxygen linkages.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1814

oxidized species

A term used to characterize the degree of oxidation (or reduction) in atoms, molecules and ions. It can be applied to an atom in a molecule or an ion which has a high oxidation state. An element or atom in a compound can be oxidized by reaction with oxygen, while it can be reduced by reaction with hydrogen. An oxidized species may be formed also through the loss of electrons (either to the positive electrode in a cell, or through transfer to another atom or group of atoms). For example, the sulfur in H_2S is reduced sulfur relative to elementary sulfur, while SO_2 and SO_3 are oxidized. Metallic iron (Fe) is a reduced state of iron, while the Fe^{2+} ion (ferrous ion) and Fe^{3+} ion (ferric ion) are oxidized states of iron. Fe^{3+} is in a higher oxidation state than Fe^{2+} which is in a higher oxidation state than Fe.
See: oxidation state

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2204

oxidoreductases

Enzymes that catalyse electron transfer in oxidation-reduction reactions. Oxidoreductases are classified into several groups according to their respective donors or acceptors.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

oxime *O*-ethers

O-Hydrocarbyl oximes $R_2C{=}NOR'$ ($R' \neq H$).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

oximes

Compounds of structure $R_2C{=}NOH$ derived from condensation of aldehydes or ketones with hydroxylamine. Oximes from aldehydes may be called aldoximes; those from ketones may be called ketoximes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

oxo carboxylic acids

Synonym: oxo acids

Compounds having a carboxy group as well as an aldehydic or ketonic group in the same molecule, e.g. $HC({=}O)CH_2CH_2CH_2C({=}O)OH$ 5-oxopentanoic acid. In an organic context the term is generally shortened to oxo acids. The full name should be used if confusion with oxoacids seems possible.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1354

oxo compounds

Compounds containing an oxygen atom, =O, doubly bonded to carbon or another element. The term thus embraces aldehydes, carboxylic acids, ketones, sulfonic acids, amides and esters. Oxo used as an adjective (and thus separated by a space) modifying another class of compound, as in oxo carboxylic acids, indicates the presence of an oxo substituent at any position. To indicate a double-bonded oxygen that is part of a ketonic structure, the term keto is sometimes used as a prefix, but such use has been abandoned by IUPAC for naming specific compounds. A traditional use of keto is for indicating oxidation of CHOH to C=O in a parent compound that contains OH groups, such as carbohydrates, e.g. 3-ketoglucose.
See: ketoaldonic acids, ketoaldoses

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1355

oxoacids

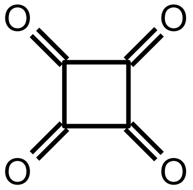
Synonym: oxyacid (oxy-acid)

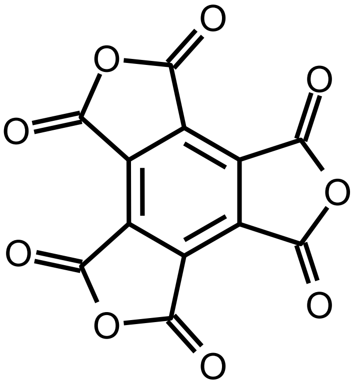
Oxoacids (and its variants oxyacids, oxo acids, oxy-acids, oxiacids, oxacids) is a traditional name for any acid having oxygen in the acidic group. The term stands in contradistinction to `hydracids' (e.g. HCl) lacking oxygen. The term oxoacid now refers to a compound which contains oxygen, at least one other element, and at least one hydrogen bound to oxygen, and which produces a conjugate base by loss of positive hydrogen ion(s) (hydrons). E.g. $P(OH)_3$, RC(=O)OH , HOSOH , HOCl , HON=O , $(HO)_2SO_2$, $RP(=O)(OH)_2$.
See also: oxo carboxylic acids

Source:
PAC, 1995, *67*, 1307 ***(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))*** on page 1355
Red Book, p. 123

oxocarbons

Compounds consisting wholly of carbon and oxygen, e.g. CO, O=C=O , O=C=C=C=O ,





Source:
PAC, 1995, *67*, 1307 ***(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))*** on page 1355

oxonium ions

The parent ion H_3O^+ and substitution derivatives thereof.
See: onium compounds

Source:
PAC, 1995, *67*, 1307 ***(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))*** on page 1355

oxonium ylides

1. Compounds having the structure $R_2O^+–C^−R_2$.
   See: ylides
2. A class of 1,3-dipolar compounds of general structure $R_2C{=}O^+–Y^−$, comprising carbonyl imides, carbonyl oxides and carbonyl ylides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1355

oxygen-flask combustion

in spectrochemical analysis

In order to determine elements which are easily volatilized, or are present as volatile species, organic material may be ashed in oxygen in a closed oxygen combustion system. One such method is oxygen-flask combustion by which the test sample is burned in a closed flask containing oxygen and an absorbing solution in which the analytes are subsequently determined.

Source:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1468

oxylium ions

Species of the form RO^+ , e.g. CH_3O^+ methoxylium, HO^+ hydroxylium.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1355

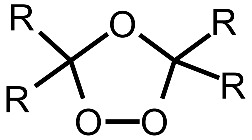
ozone hole

A region of the stratosphere over Antarctica in which a marked decrease in the concentration of ozone has been observed in the Antarctic spring in recent years. The origin of this phenomenon is not yet established, but several theories based on both physical (transport related) and chemical processes (involvement of the halocarbons and their products of oxidation) have been suggested. The latter explanation appears to be in better accord with recent findings.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2205

ozonides

The 1,2,4-trioxolanes formed by the reaction of ozone at a carbon–carbon double bond, or the analogous compounds derived from acetylenic compounds.



See: molozonides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1355

π – π* state

An excited state related to the ground state by a π → π* transition.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

π → π* transition

An electronic transition described approximately as a promotion of an electron from a 'bonding' π orbital to an 'antibonding' π orbital designated as π*.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

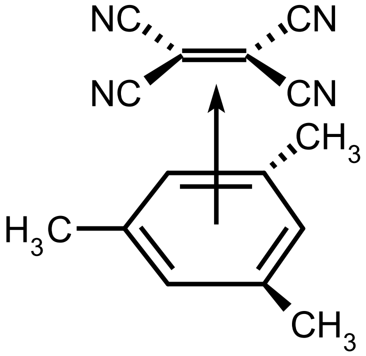
π → σ* transition

An electronic transition described approximately as a promotion of an electron from a 'bonding' orbital π to an 'antibonding' orbital σ designated as σ*. Such transitions generally involve high transition energies and appear close to or mixed with Rydberg transitions.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

π-adduct

An adduct formed by electron-pair donation from a π-orbital into a σ-orbital, or from a σ-orbital into a π-orbital, or from a π-orbital into a π-orbital. For example:



Such an adduct has commonly been known as a 'π-complex', but, as the bonding is not necessarily weak, it is better to avoid the term complex.
See also: coordination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1154
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

π-bond

See: σ, π

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1163

π-complex [obsolete]

See: π-adduct

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1154
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1312

π-electron acceptor/donor group

A substituent capable of a +R (e.g. NO_2) or −R (e.g. OCH_3) effect, respectively.
See: electronic effect, polar effect, σ-constant

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1155

packed column

in chromatography

A tube containing a solid packing.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831

packing

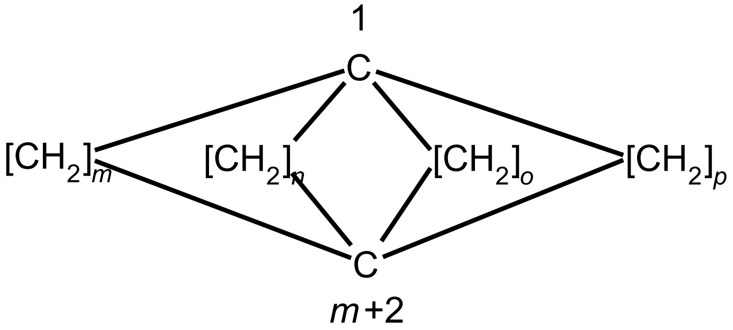
in column chromatography

The active solid, stationary liquid plus solid support, or swollen gel put in the column. The term packing refers to the conditions existing before the chromatographic run is started (i.e. to the material introduced into the column), whereas the stationary phase refers to the conditions during the run.
See also: totally porous packing, pellicular packing

Source:
Orange Book, p. 97
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831

paddlanes

Tricyclic saturated hydrocarbons having two bridgehead carbon atoms joined through four bridges, systematically named tricyclo [$m.n.o.p^{1,(m+2)}$]alkanes, have been referred to as [$m.n.o.p$]paddlanes (when $p = 0$, the compounds are propellanes).



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1355

pair attenuation coefficient

in nuclear chemistry

The attenuation coefficient when only the pair production process is taken into account.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

pair correlation length, ξ

in thin films

A quantity which approximates to the characteristic length associated with certain number density profiles of diffuse layers. ξ is defined as the separation between two interacting entities (molecules, macromolecular segments, ions, spins), either in bulk or interfacial regions, beyond which an appropriate function, referred to as pair correlation function, either decays (e.g. to $\frac{1}{e}$ of an 'initial' value) or vanishes. A characteristic length must be confused neither with the effective thickness of the interfacial layer, nor with the range (effective distance) of the intermolecular (pair) potential. This range is defined by the distance over which this potential and the corresponding correlation function both vanish.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1674

pair production

in nuclear chemistry

The simultaneous formation of an electron and a positron as a result of the interaction of a photon of sufficient energy ($> 1.02\ \mathrm{MeV}$) with the field of a particle.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

Pallmann effect

Synonymous with suspension effect *in an ion-selective electrode*

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2533

PAN-based carbon fibres

Carbon fibres obtained from polyacrylonitrile (PAN) precursor fibres by stabilization treatment, carbonization and final heat treatment.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 499

paraffin [obsolete]

Obsolescent term for saturated hydrocarbons, commonly but not necessarily acyclic. Still widely used in the petrochemical industry, where the term designates acyclic saturated hydrocarbons, and stands in contradistinction to naphthenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1356

parallel reactions

See: composite reaction, simultaneous reactions

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2293
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2297
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1098

parallel-chain crystal

in polymers

A type of crystal resulting from parallel packing of stems, irrespective of the stems' directional sense.

Source:
Purple Book, p. 84

paramagnetic

Substances having a magnetic susceptibility greater than 0 are paramagnetic. They are drawn into a magnetic field.
See also: diamagnetic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1149

parametric amplification

Amplification of a signal based on parametric processes.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 380

parametric processes

Synonym: optical parametric processes

Interaction of photons in a non-linear medium satisfying the energy and momentum conservation laws. During the interaction the photon frequencies are mixed and photon(s) with different frequencies are created.
Note:
Optical parametric processes of three interacting beams, called frequency mixing processes, are: second-harmonic generation (SHG), sum-frequency generation (SFG), difference-frequency generation (DFG), optical parametric generation and amplification (OPG and OPA), and optical parametric oscillation (OPO).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 381

parent hydride

An unbranched acyclic or cyclic structure or an acyclic/cyclic structure having a semisystematic or trivial name to which only hydrogen atoms are attached.

Source:
Blue Book (Guide), p. 13

parent ion

in mass spectrometry

An electrically charged molecular moiety which may dissociate to form fragments, one or more of which may be electrically charged, and one or more neutral species. A parent ion may be a molecular ion or an electrically charged fragment of a molecular ion.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549
Orange Book, p. 205

Pariser–Parr–Pople (PPP) method

A semi-empirical quantum mechanical method of calculation of the properties of conjugated molecules and ions from self-consistent-field theory and the π-electron approximation.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1956

partial anodic (cathodic) current

When a single electrochemical reaction occurs at an electrode (i.e. all other electrochemical reactions may be neglected):

$$I = I_\mathrm{a} + I_\mathrm{c}$$

where I is the total current, I_a is the positive partial anodic current and I_c is the negative partial cathodic current. When more than one reaction is significant the reactions may be numbered and the numbers used as subscripts: $I_{1,\mathrm{a}}$, $I_{1,\mathrm{c}}$, $I_{2,\mathrm{a}}$, etc. Then:

$$I = \sum I_{i,\mathrm{a}} + \sum I_{i,\mathrm{c}}$$

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 512

partial charge exchange reaction

Synonymous with partial charge transfer reaction.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1556

partial charge transfer reaction

An ion/neutral species reaction wherein the charge on a multiply-charged reactant ion is reduced.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1556

partial decay constant

in nuclear chemistry

For a radionuclide: the probability in unit time for the decay of one of its nuclei by one of several modes of decay.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

partial digestion

Also contains definition of: selective digestion *in spectrochemical analysis*

in spectrochemical analysis

In partial digestion and/or selective digestion procedures only part or some of the analytes present are brought into solution. This may be preferred to total decomposition if relative concentrations of the analyte in the test samples provide sufficient information (e.g. materials for geochemical exploration).

Source:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1469

partial isotherm (or individual isotherm)

in surface chemistry

The function relating, at constant temperature and pressure, the amount of a particular component in the interfacial layer per unit area (or per unit mass of adsorbent) with its mole fraction (or concentration) in the liquid phase. This function can be evaluated only when the location and the thickness of the interfacial layer have been defined.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 594

partial kinetic current

in electrochemistry

The current which would flow if mass transport were infinitely fast.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 515

partial least squares (PLS)

Partial least squares projection to latent structures (*PLS*) is a robust multivariate generalized regression method using projections to summarize multitudes of potentially collinear variables.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1148

partial mass density, ρ_{B}

Change in mass due to addition of a small amount of component to a system divided by the change in volume of the system. The systematic name is partial volumic mass.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 986

partial microscopic diffusion control (encounter control)

See: microscopic diffusion control (encounter control)

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 173

partial molar Gibbs energy

See: chemical potential

Source:
Green Book, 2nd ed., p. 49

partial molar quantity

Change in the considered extensive quantity when an infinitesimal amount of substance is added to the system at constant temperature, pressure and amounts of all other constituents of the system divided by the added amount.

Source:
Green Book, 2nd ed., p. 49

partial pressure

See: pressure

Source:
Green Book, 2nd ed., p. 12
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 538

partial rate factor

The rate of substitution at one specific site in an aromatic compound relative to the rate of substitution at one position in benzene. For example, the partial rate factor f_p^{Z} for *para*-substitution in a monosubstituted benzene C_6H_5Z is related to the rate constants $k(\mathrm{C_6H_5Z})$ and $k(\mathrm{C_6H_6})$ for the total reaction (i.e. at all positions) of C_6H_5Z and benzene, respectively, and % *para* (the percentage *para*-substitution in the total product formed from C_6H_5Z) by the relation:

$$f_p^{\mathrm{Z}} = \frac{6\,k(\mathrm{C_6H_5Z})}{k(\mathrm{C_6H_6})}\,\frac{\%\ \mathrm{para}}{100}$$

Similarly for *meta*-substitution:

$$f_m^{\mathrm{Z}} = \frac{6\,k(\mathrm{C_6H_5Z})}{2\,k(\mathrm{C_6H_6})}\,\frac{\%\ \mathrm{meta}}{100}$$

(The symbols p_f^Z, m_f^Z, o_f^Z are also in use.) The term applies equally to the *ipso* position, and it can be extended to other substituted substrates undergoing parallel reactions at different sites with the same reagent according to the same rate law.
See also: selectivity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1149

partial specific volume, v_B

Change in volume of a system when a small amount of component is added divided by the mass of the added component. The systematic name is partial massic volume.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 986

partially draining

An adjective describing a chain macromolecule that behaves in a hydrodynamic field as though the solvent within the domain of the macromolecule were progressively more immobilized with respect to the macromolecule in the direction from its outer fringes inward. A freely draining macromolecule and a non-draining macromolecule are two extremes of the concept of a partially draining macromolecule.

Source:
Purple Book, p. 61

particle concentration

in atmospheric chemistry

Commonly expressed in several ways: mass concentration (usually as $\mu g\ m^{-3}$) or number concentration (number of particles cm^{-3}); modern instrumentation allows measurement of the number of particles as a function of size as well as the total number present in a given air volume. For atmospheric aerosols, this is a complex distribution for which diameters range from below 0.01 to above $100\ \mu m$; the particles making the highest contribution to the total number density are in the size range below $0.1\ \mu m$, those contributing most to the total surface area are in the 0.1 to $1.0\ \mu m$ range, while those with the highest contribution to the volume or mass of the aerosol come from both the 0.1 to $1.0\ \mu m$ and 1.0 to $100\ \mu m$ ranges.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2181

particle density

in nuclear chemistry

The number of particles (nuclear or elementary) divided by the containing volume.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

particle induced X-ray emission analysis

A kind of analysis based on the measurement of the energies and intensities of characteristic X-radiation emitted by a test portion during irradiation with charged particles other than electrons.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

particle scattering function

Synonym: particle scattering factor

The ratio of the intensity of radiation scattered at an angle of observation θ to the intensity of radiation scattered at an angle zero, i.e. $P(\theta) \equiv \frac{R(\theta)}{R(0)}$. An alternative recommended symbol is P_{θ}. Synonymous with particle scattering factor.

Source:
Purple Book, p. 66

particle size distribution

in atmospheric chemistry

The size of the liquid or solid particles in the atmosphere usually extends from > 0.01 to $< 100\ \mu\text{m}$ in diameter. In the earth's atmosphere the distribution function which describes the number of particles as a function of diameter, mass or surface area of the aerosol can be determined reasonably well with modern instrumentation.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2205

particle size

in atmospheric chemistry

To describe the size of liquid or solid particles (aerosol) the average or equivalent diameter is used. For non-spherical particles collected in an impactor, for example, the aerodynamic diameter of a particle of arbitrary shape and density refers to the size of a spherical particle of unit density that would deposit on a given impactor surface.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2205

particular property

A property of a given object (phenomenon, body or substance). 'Particular property' includes the concept of particular quantity. The adjective 'particular' may be omitted, if no ambiguity is caused.
See also: property

Source:
PAC, 1995, *67*, 1563 *(Properties and units in the clinical laboratory sciences-I. Syntax and semantic rules (IUPAC-IFCC Recommendations 1995))* on page 1565

particulate carbon

A carbon material consisting of separated monolithic particles.
Note:
Distinctions should be made between coarse particulate carbon or granular carbon (larger than about $100\ \mu\text{m}$, but smaller than about $1\ \text{cm}$ in average size), fine particulate carbon or powder or flour (between 1 and $100\ \mu\text{m}$ in average size) and colloidal carbon (below approximately $1\ \mu\text{m}$ in size in at least one direction), e.g. carbon blacks and colloidal carbon.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 499

particulate gel

Gel in which the network component comprises solid particles.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1807

particulate matter

in atmospheric chemistry

A general term used to describe airborne solid or liquid particles of all sizes. The term aerosol is recommended for general use in describing airborne particulate matter.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2205

particulate sol

Sol in which the dispersed phase consists of solid particles.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1806

partition

This term is often used as a synonym for distribution and extraction. However, an essential difference exists by definition between distribution constant or partition ratio and partition constant. The term partition should be, but is not invariably, applied to the distribution of a single definite chemical species between the two phases.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2378

partition chromatography

Chromatography in which separation is based mainly on differences between the solubility of the sample components in the stationary phase (gas chromatography), or on differences between the solubilities of the components in the mobile and stationary phases (liquid chromatography).

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 826
Orange Book, p. 94

partition coefficient [obsolete]

This term is not recommended and should not be used as a synonym for partition constant, partition ratio or distribution ratio.
See also: distribution constant

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2385
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 986

partition constant, $K_{\mathrm{D}}^{\mathrm{o}}$

The ratio of activity of a given species A in the extract to its activity in the other phase with which it is in equilibrium, thus:

$$(K_D^o)_A = \frac{a_{A,org}}{a_{A,aq}}$$

Its value should not vary with composition but depends on the choice of standard states and on the temperature (and eventually the pressure).
See: transfer activity coefficient, distribution constant

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2385

partition function

For a molecule the ratio of the total number of molecules to their number in the non-degenerate ground state.

Source:
Green Book, 2nd ed., p. 39

partition isotherm

in chromatography

Isotherm describing partition of the sample component between the bulk of a liquid stationary phase and a liquid, gaseous or supercritical mobile phase.

Source:
PAC, 1996, *68*, 1591 *(Nomenclature for non-linear chromatography (IUPAC Recommendations 1996))* on page 1592

partition ratio, K_D

The ratio of the concentration of a substance in a single definite form, A, in the extract to its concentration in the same form in the other phase at equilibrium, e.g. for an aqueous/organic system:

$$(K_D)_A = \frac{[\,A\,]_{org}}{[\,A\,]_{aq}}$$

Notes:

1. K_D is sometimes called the distribution constant; this is a good synonym. The terms distribution coefficient, distribution ratio, partition constant and extraction constant should not be used as synonyms for partition ratio.
2. The use of the inverse ratio (aqueous/organic) may be appropriate in certain cases, e.g. where the organic phase forms the feed but its use in such cases should be clearly specified. The ratio of the concentration in the denser phase to the less dense phase is not recommended as it can be ambiguous.
3. If the pure solvent and infinitely dilute feed are taken as the standard states, $K_D \rightarrow K_D{}^\circ$ as the total concentration of dissolved materials decreases.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2385

pascal

SI derived unit of pressure, $\mathrm{Pa} = \mathrm{N\ m^{-2}} = \mathrm{kg\ m^{-1}\ s^{-2}}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 986

passivation

in electrochemical corrosion

The process of transition from the active to the passive state by formation of the passivating film. Passivation is achieved by an anodic current which at the respective electrode potential must be larger than the maximum current, or by the presence of an oxidized substance in the neighbouring solution which passivates by being reduced (passivator).
See also: passive state, active state

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

passivation potential

in electrochemical corrosion

The most negative electrode potential at which the passivating film is formed. The passivation potential is equal to or more positive than the equilibrium potential of formation of the phase constituting the film. Usually, the corrosion current goes through a maximum at the passivation potential.
See also: corrosion, passive state

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

passive metal

A metal corroding in the passive state.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

passive sampler

A device for preconcentration of trace substances from gaseous media based on molecular diffusion without controlled conveyance of the gas to be investigated (e.g. work place air).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2205

passive state

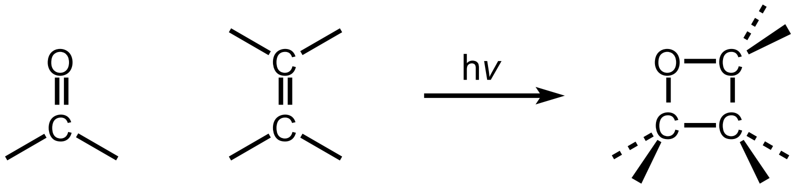
in electrochemical corrosion

The passive state is characterized by a contiguous 'passivating film' of solid corrosion products separating the metallic phase from the adjacent electrolyte. Corrosion in the passive state involves growth of the passivating film and/or transfer of metal ions through the film into the electrolyte.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

Paterno–Büchi reaction

The photocycloaddition of an electronically excited carbonyl group to a ground state olefin yielding an oxetane.



Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2258

pattern recognition

Pattern recognition is the identification of patterns in large data sets, using appropriate mathematical methodology. Examples are principal component analysis (*PCA*), *SIMCA*, partial least squares (*PLS*) and artificial neural networks (*ANN*).

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1148

paucidisperse system

A colloidal system in which only a few particle-sizes occur.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

Pauli exclusion principle

A rule, complementary to the aufbau principle, of building up the electronic configuration of atoms and molecules: a maximum of two electrons can occupy an orbital and then only providing that the spins of the electrons are paired, i.e. opposed. The principle demands that the wavefunction for a many-electron system must be asymmetric with respect to the permutation of the space-spin coordinates for every pair of electrons.
Note:
See also: antisymmetry principle.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1956

peak analysis

The extraction of relevant peak parameters (i.e. position, area) from a measured spectrum.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522
PAC, 1982, *54*, 533 *(The structure and intramolecular mobility of macromolecules in solution as studied by polarized luminescence)* on page 547

peak area

in chromatography

The area enclosed between the peak and the baseline.

Source:
Orange Book, p. 101

peak area method

A kind of peak analysis in which a peak area is calculated by subtracting an estimate of the underlying continuum in a relevant part of a measured spectrum.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523

peak base

in chromatography

The interpolation, in a differential chromatogram, of the baseline between the extremities of the peak.

Source:
Orange Book, p. 101

peak concentration (trace atmospheric component)

The highest concentration of a given trace component which was measured with a continuous analyser during a specified sampling period.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2205

peak current

In linear-sweep voltammetry, triangular-wave voltammetry, cyclic triangular-wave voltammetry, and similar techniques, the maximum value of the faradaic current due to the reduction or oxidation of a substance B during a single sweep. This maximum value is attained after an interval during which the concentration of B at the electrode-solution interface decreases monotonically, while the faradaic current due to the reduction or oxidation of B increases monotonically, with time. It is attained before an interval during which this current decreases monotonically with time because the rate of transport of B toward the electrode-solution interface is smaller than the rate at which it is removed from the interface by electrolysis. The term has also been used to denote the maximum value of the faradaic current attributable to the reduction or oxidation of an electroactive substance in techniques such as ac polarography, differential pulse polarography, and derivative polarography. However, these techniques give curves that arise in ways different from that cited above, and the terms summit, summit current, and summit potential are therefore recommended for use in connection with such techniques.
See also: apex current

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1498
Orange Book, p. 56

peak elution volume (time), $\bar{V}_{\mathrm{R}}$, $\bar{t}_{\mathrm{R}}$

in column chromatography

The volume of mobile phase entering the column between the start of the elution and the emergence of the peak maximum, or the corresponding time. In most of the cases, this is equal to the total retention volume (time). There are, however, cases when the elution process does not start immediately at sample introduction. For example, in liquid chromatography, sometimes the column is washed with a liquid after the application of the sample to displace certain components which are of no interest and during this treatment the sample does not move along the column. In gas chromatography, there are also cases when a liquid sample is applied to the top of the column but its elution starts only after a given period. This term is useful in such cases.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 841

Orange Book, p. 104

peak enthalpimetry [obsolete]

See: flow injection enthalpimetry

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2491

peak fitting

A kind of peak analysis in which a relevant part of a spectrum is fitted with a theoretical response function.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523
Orange Book, p. 234

peak height

in chromatography

The distance between the peak maximum and the peak base, measured in a direction parallel to the axis representing the detector response.

Source:
Orange Book, p. 102

peak

Also contains definition of: unresolved peak *in chromatography*

in chromatography

The portion of a differential chromatogram recording the detector response when a single component is eluted from the column. If separation is incomplete, two or more components may be eluted as one unresolved peak.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 835
Orange Book, p. 96
Orange Book, p. 101

peak maximum

in chromatography

The point on the peak at which the distance to the peak base, measured in a direction parallel to the axis representing the detector response, is a maximum.

Source:
Orange Book, p. 102

peak potential

In linear-sweep voltammetry, triangular-wave voltammetry, cyclic triangular-wave voltammetry, and similar techniques, the potential of the indicator electrode at which the peak current is attained.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1502

peak resolution, R_s

in chromatography

The separation of two peaks in terms of their average peak width at base ($t_{R2} > t_{R1}$):

$$R_s = \frac{t_{R2} - t_{R1}}{\frac{w_{b1} + w_{b2}}{2}} = \frac{2\,(t_{R2} - t_{R1})}{w_{b1} + w_{b2}}$$

In the case of two adjacent peaks it may be assumed that $w_{b1} \approx w_{b2}$, and thus, the width of the second peak may be substituted for the average value:

$$R_s \approx \frac{t_{R2} - t_{R1}}{w_{b2}}$$

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 847
Orange Book, p. 108

peak widths

in chromatography

Peak widths represent retention dimensions (time or volume) parallel to the baseline. If the baseline is not parallel to the axis representing time or volume, then the peak widths are to be drawn parallel to this axis. Three peak-width values are commonly used in chromatography. Peak width at base (w_b) is the segment of the peak base intercepted by the tangents drawn to the inflection points on either side of the peak. Peak width at half height (w_h) is the length of the line parallel to the peak base at 50% of the peak height that terminates at the intersection with the two limbs of the peak. Peak width at inflection points (w_i) is the length of the line drawn between the inflection points parallel to the peak base. The peak width at base may be called the 'base width'. However, the peak width at half height must never be called the 'half width' because that has a completely different meaning. Also, the symbol $w_{1/2}$ should never be used instead of w_h.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 836
Orange Book, p. 101
Orange Book, p. 102

pectins

Polyuronic acids mostly derived from D-galacturonic acid (abundant in some fruits).
See also: uronic acids

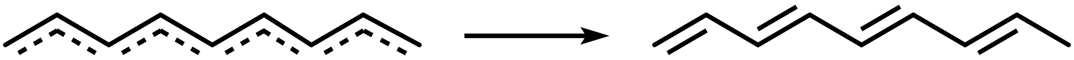
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1356

Peierls distortion

Distortion of a regular one-dimensional structure with a partially occupied band to give bond alternation, eventually leading to dimerization or oligomerization. The degree of oligomerization, λ depends on the electronic population of the conduction band indicated by the wave vector of the Fermi level k_F

$$\lambda = 2\,\pi / k_F$$

Note:
A Peierls distortion opens a gap at the Fermi level, producing a net stabilization of the distorted structure. The Peierls distortion for chain compounds is analogous to the Jahn–Teller effect for molecules. The prototypical example of the Peierls distortion in organic chemistry is the bond alternation present in polyvinylene.



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 381

Peierls transition

A metal-insulator transition in quasi one-dimensional solids that occurs as a result of a band gap opening up at the Fermi energy due to a displacive distortion of the regular array increasing the unit cell length, usually a dimerization; the decrease in electronic energy outweighs the increase in lattice energy. Example: The transition in methylethylmorpholinium tetracyanoquinodimethanide at 335 K.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

pellicular packing

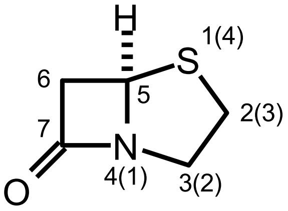
in chromatography

In this case the stationary phase forms a porous outer shell on an impermeable particle.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831

penams

Natural and synthetic antibiotics containing the 4-thia-1-azabicyclo[3.2.0]heptan-7-one structure, generally assumed to have the 5*R* configuration unless otherwise specified. The numbering of the penam skeleton differs from that of the von Baeyer named bicyclic system. Where they differ the von Baeyer numbering is shown in parentheses in the example.



See also: penems

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1356

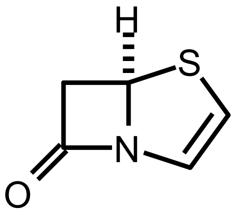
pendant group (side group)

An offshoot, neither oligomeric nor polymeric from a chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2297

penems

2,3-Didehydropenams.



See: penams

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1356

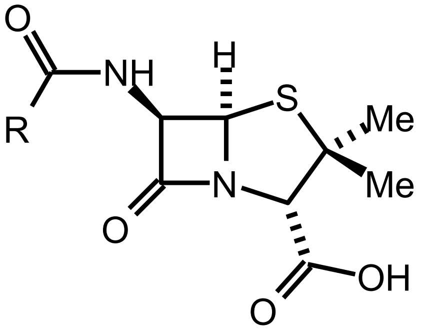
penetrant (permeant)

Entity from a phase in contact with one of the membrane surfaces that passes though the membrane.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1484

penicillins

Substituted penams having the basic structure shown, including the natural penicillins and synthetic analogues.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1356

Penning gas mixture

A Penning gas mixture consists of a rare gas containing impurity atoms possibly at very low concentrations. The impurity atoms have an ionization potential V_{ion} which is lower than or equal to the metastable potential (V_{meta}) of the parent noble gas. The Penning effect in a Penning gas mixture is the ionization by charge transfer (charge exchange) during collision between a metastable atom and a neutral atom which decreases the average energy to form an ion pair, e.g.

$$\mathrm{Cu} + \mathrm{Ar}_{\mathrm{meta}} \longrightarrow \mathrm{Cu}^{+} + \mathrm{Ar} + \mathrm{e}^{-1}$$

In a glow discharge, this results in an increase of the the ionization coefficient (Townsend first coefficient), a decrease in breakdown potential and a lowering of the cathode fall potential. The magnetic Penning effect describes the increase of the ionization probability of gas in a low pressure electrical discharge resulting from the helical (spiral) movement of electrons in a magnetic field placed normal to the anode-cathode electrical field.

Source:
Orange Book, p. 148

pentads

in polymers

See: constitutional sequence

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2299

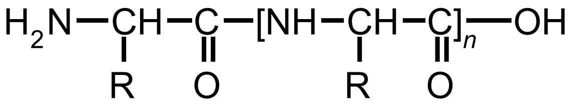
pentaprismo-

An affix used in names to denote ten atoms bound into a pentagonal prism.

Source:
Red Book, p. 245
Blue Book, p. 465

peptides

Amides derived from two or more amino carboxylic acid molecules (the same or different) by formation of a covalent bond from the carbonyl carbon of one to the nitrogen atom of another with formal loss of water. The term is usually applied to structures formed from α-amino acids, but it includes those derived from any amino carboxylic acid.



$$\mathrm{H_2N{-}}\underset{\displaystyle \mathrm{R}}{\underset{|}{\mathrm{CH}}}\mathrm{{-}}\underset{\displaystyle \mathrm{O}}{\underset{\|}{\mathrm{C}}}\mathrm{{-}[NH{-}}\underset{\displaystyle \mathrm{R}}{\underset{|}{\mathrm{CH}}}\mathrm{{-}}\underset{\displaystyle \mathrm{O}}{\underset{\|}{\mathrm{C}}}\mathrm{]}_{n}\mathrm{{-}OH}$$

(R may be any organyl group, commonly but not necessarily one found in natural amino acids)
See also: proteins, retro, carboxylic acids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1356
White Book, p. 48

peptidoglycan

A glycosaminoglycan formed by alternating residues of D-glucosamine and either muramic acid {2-amino-3-*O*-[(*S*)-1-carboxyethyl]-2-deoxy-D-glucose} or L-talosaminuronic acid (2-amino-2-deoxy-L-taluronic acid), which are usually *N*-acetylated or *N*-glycoloylated. The carboxyl group of the muramic acid is commonly substituted by a peptide containing residues of both L- and D-amino acids, whereas that of L-talosaminuronic acid is substituted by a peptide consisting of L-amino acids only.

Source:
PAC, 1988, *60*, 1389 *(Nomenclature of glycoproteins, glycopeptides and peptidoglycans (Recommendations 1985))* on page 1391
White Book, p. 85

peptization

Also contains definition of: deflocculation

Reversal of coagulation or flocculation, i.e., the dispersion of agglomerates to form a colloidally stable suspension or emulsion.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1824

per acids [obsolete]

An ambiguous term, which may imply either a higher oxidation state of a central atom, as in perchloric acid, or a derivative of hydrogen peroxide, as in $CH_3C(=O)OOH$. Accordingly, it is not recommended as a class name.
See: peroxy acids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1356

percent

One part in a hundred, $\% = 0.01$.

Source:
Green Book, 2nd ed., p. 77

percentage error

See: percentage relative error

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 601

percentage exposed

in metallic catalysts

The accessibility of the atoms of metal in metallic catalysts, supported or unsupported, depends upon the percentage of the total atoms of metal which are surface atoms. It is recommended that the term percentage exposed be employed for this quantity rather than the term dispersion which has been frequently employed.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

percentage relative error, e_{r} (%)

The relative error expressed in percent. It can be calculated from the relative error by multiplying by 100. Comment: The term 'percentage relative error' should always be quoted in full, rather than 'error' or 'percentage error' to avoid confusion.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 601

percentage standard deviation, s_{r} (%), σ_{r} (%)

The value of the relative standard deviation, expressed in percent. It can be calculated from the relative standard deviation by multiplying by 100. Comment: It is recommended that the 'relative standard deviation' be reported, rather than the 'percentage standard deviation', in order to avoid confusion where results themselves are expressed as percentages. The term 'coefficient of variation' in place of 'relative standard deviation' is not recommended.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 601

perfect network

Also contains definition of: perfect polymer network

Polymer network composed of chains all of which are connected at both of their ends to different junction points.
Note:
If a perfect network is in the rubbery state then, on macroscopic deformation of the network, all of its chains are elastically active and display rubber elasticity.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1815

perfectly polarized interphase

Differences from the behaviour of interphases containing only neutral species arise when the interphase may be described as perfectly polarized. This term is used when no charged component is common to both phases adjoining the interphase. This may arise as a result of the equilibrium conditions or from the kinetics of charge transfer and leads to an interphase impermeable to electric charge.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1260

perfusion stationary phase (material)

in liquid chromatography

Stationary phase in which the mobile phase primarily travels through the pores of the stationary phase.

Source:
PAC, 1997, *69*, 1475 *(Classification and characterization of stationary phases for liquid chromatography: Part I. Descriptive terminology (IUPAC Recommendations 1997))* on page 1479

pericyclic reaction

A chemical reaction in which concerted reorganization of bonding takes place throughout a cyclic array of continuously bonded atoms. It may be viewed as a reaction proceeding through a fully conjugated cyclic transition state. The number of atoms in the cyclic array is usually six, but other numbers are also possible. The term embraces a variety of processes, including cycloadditions, cheletropic reactions, electrocyclic reactions, sigmatropic rearrangements, etc. (provided they are concerted).
See also: multi-centre reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1150

perikinetic aggregation

in colloids

The rate of aggregation is in general determined by the frequency of collisions and the probability of cohesion during collision. If the collisions are caused by Brownian motion, the process is called perikinetic aggregation.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

period, T

Time for one cycle of a periodic phenomenon.

Source:
Green Book, 2nd ed., p. 11
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 986

periodic copolymer

A copolymer consisting of macromolecules comprising more than two species of monomeric units in regular sequence.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2301

periodic copolymerization

A copolymerization in which a periodic copolymer is formed.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2307

periodic voltage

This general term is applicable to square, triangular, and other wave forms.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1505

peripheral atom

in organic reaction mechanisms

A secondary reference (non-core) atom which at some point in the mechanistic sequence is situated in the molecule containing the core atom(s).

Source:
PAC, 1989, *61*, 23 *(System for symbolic representation of reaction mechanisms (Recommendations 1988))* on page 27

periselectivity

The differentiation between two symmetry-allowed processes, for example the [2+4] vs. [4+6] cycloaddition of cyclopentadiene to tropone.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1150

peritectic reaction

Synonym: incongruent reaction

An isothermal, reversible reaction between two phases, a liquid and a solid, that results, on cooling of a binary, ternary, ... , n system in one, two, ... $(n - 1)$ new solid phases. Synonymous with incongruent reaction.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

peritectoid reaction

Synonym: metatectoid reaction

An isothermal, reversible reaction in the solid state, that, on cooling of a binary, ternary, ... , n system, results in one, two, ... $(n - 1)$ new solid phases. For example, in a binary system containing two solids $\alpha^{'}$ and $\alpha^{''}$

$$\alpha^{'} + \alpha^{''} \rightarrow \beta$$

Synonymous with metatectoid reaction.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

peritectoid temperature

The maximum temperature at which a peritectoid reaction can occur.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

permanent crosslink

Crosslink formed by covalent bonds, intermolecular or intramolecular interactions that are stable under the conditions of use of the material formed.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1819

permeability, μ

Permeability of vacuum multiplied by the relative permeability.

Source:
Green Book, 2nd ed., p. 15

permeability of vacuum, μ_0

Fundamental physical constant by definition equal to $4\,\pi \times 10^{-7}\ \mathrm{H\ m^{-1}}$, exactly.

Source:
Green Book, 2nd ed., p. 15

permeate

Stream containing penetrants that leaves a membrane module.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1484

permeation chromatography

Also contains definition of: gel permeation chromatography

Separation based mainly upon exclusion effects, such as differences in molecular size and/or shape (e.g. molecular-sieve chromatography) or in charge (e.g. ion-exclusion chromatography). The term gel-permeation chromatography is widely used for the process when the stationary phase is a gel. The term gel-filtration is not recommended.

Source:
Orange Book, p. 94

permeation tube

A device used for dynamic preparation of test gas mixtures by means of controlled permeation of a gaseous analyte out of a container through polymer material into a carrier gas stream. These devices containing certain condensable gases (e.g. NO_2 , SO_2 , etc.) when operated at closely controlled temperatures can be used as primary standards calibrated in terms of the weight loss per unit time.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2205

permittivity, ε

Permittivity of vacuum multiplied by the relative permittivity.

Source:
Green Book, 2nd ed., p. 14

permittivity of vacuum

Fundamental physical constant $\varepsilon_0 = \frac{1}{\mu_0 {c_0}^2}$ exactly, where μ_0 is the permeability of vacuum and c_0 the speed of light in vacuum. It is equal to $8.854\ 187\ 817\ ... \times 10^{-12}\ \mathrm{F\ m^{-1}}$.

Source:
CODATA 2006
Green Book, 2nd ed., p. 14

permselectivity

A term used to define the preferential permeation of certain ionic species through ion-exchange membranes.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 856

peroxides

Compounds of structure ROOR in which R may be any organyl group (The term is also used in an inorganic sense to denote salts of the anion ${O_2}^{2-}$).
See also: hydroperoxides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1356

peroxisome

Organelle, similar to a lysosome, characterized by its content of catalase (EC 1.11.1.6), peroxidase (EC 1.11.1.7) and other oxidative enzymes.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2080

peroxy acids

Acids in which an acidic –OH group has been replaced by an –OOH group, e.g. $CH_3C(=O)OOH$ peroxyacetic acid, $PhS(=O)_2OOH$ benzeneperoxysulfonic acid.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1356

perpendicular effect

See: More O'Ferrall–Jencks diagram

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1150

persistence length

in polymers

The average projection of the end-to-end vector on the tangent to the chain contour at a chain end in the limit of infinite chain length. The persistence length (symbol a) is the basic characteristic of the worm-like chain.

Source:
Purple Book, p. 51

persistent

A term used to characterize radicals which have lifetimes of several minutes or greater in dilute solution in inert solvents. Persistence is a kinetic or reactivity property. In contrast, radical stability, which is a thermodynamic property, is expressed in terms of the C–H bond strength of the appropriate hydrocarbon. The lifetime of a radical is profoundly influenced by steric shielding of the radical centre by bulky substituents.
See also: transient

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1150

perspective formula

A geometric representation of stereochemical features of a molecule or model which appears as a view from an appropriate direction.
See: Fischer projection, Newman projection, projection formula, saw-horse projection, wedge projection, zig-zag projection
See also: stereochemical formula

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2213

perstraction

Separation process in which membrane permeation and extraction phenomena occur by contacting the downstream with an extracting solvent.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1484

perturbation theory

Along with variational method, the second major quantum-mechanical approximation method. The methods of perturbation theory are based on representation of the Hamiltonian of a system under study, $\boldsymbol{H}$, through the Hamiltonian, $\boldsymbol{H}^0$, of a system, whose Schroedinger equation is solvable, and its relatively small perturbation $\boldsymbol{H}^{'}$: $\boldsymbol{H} = \boldsymbol{H}^0 + \boldsymbol{H}^{'}$. Numerous techniques are derived allowing one to relate the unknown eigenvalues and eigenfunctions of the perturbed system to the known eigenvalues and eigenfunctions of the unperturbed system. As distinct from the variational method, the methods of perturbation theory are applicable to all the electronic states of an atom or molecule. When $\boldsymbol{H}^{'}$ is time-dependent, the perturbed system does not have stationary states. In this case time-dependent perturbation theory, which is the method of approximate calculation of the expansion of wave-functions of the perturbed system over wave-functions of stationary states of the unperturbed system, must be employed. The applications of this method are associated mostly with studies of light emission and absorption by atoms and molecules.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1957

perturbed dimensions

in polymers

The dimensions of an actual polymer random coil not in a theta state.

Source:
Purple Book, p. 48

pervaporation

Membrane-based process in which the feed and retentate streams are both liquid phases while permeant emerges at the downstream face of the membrane as a vapour.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1488

pesticide

Strictly, a substance intended to kill pests: in common usage, any substance used for controlling, preventing, or destroying animal, microbiological or plant pests.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2081

pesticide residue

Any substance or mixture of substances in food for man or animals resulting from the use of a pesticide including any specified derivatives, such as degradation and conversion products, metabolites, reaction products and impurities considered to be of toxicological significance.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2081

peta

SI prefix for 10^{15} (symbol: P).

Source:
Green Book, 2nd ed., p. 74

petroleum coke

A carbonization product of high-boiling hydrocarbon fractions obtained in petroleum processing (heavy residues). It is the general term for all special petroleum coke products such as green, calcined and needle petroleum coke.
Note:
High-boiling hydrocarbon fractions (heavy residues) used as feedstock for petroleum coke are residues from distillation (atmospheric pressure, vacuum) or cracking (e.g. thermal, catalytic, steam-based) processes. The nature of feedstock has a decisive influence on the graphitizability of the calcined coke.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 499

petroleum pitch

A residue from heat treatment and distillation of petroleum fractions. It is solid at room temperature, consists of a complex mixture of numerous predominantly aromatic and alkyl-substituted aromatic hydrocarbons, and exhibits a broad softening range instead of a defined melting temperature.
Note:
The hydrogen aromaticity (ratio of aromatic to total hydrogen atoms) varies between 0.3 and 0.6. The aliphatic hydrogen atoms are typically present in alkyl groups substituted on aromatic rings or as naphthenic hydrogen.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 499

pH

The quantity pH is defined in terms of the activity of hydrogen(1+) ions (hydrogen ions) in solution:

$$\mathrm{pH} = -\lg[a(\mathrm{H}^+)] = -\lg[m(\mathrm{H}^+)\,\gamma_\mathrm{m}(\mathrm{H}^+)\,/\,m^\ominus]$$

where $a(\mathrm{H}^+)$ is the activity of hydrogen ion (hydrogen 1+) in aqueous solution, $\mathrm{H}^+(\mathrm{aq})$, $\gamma_\mathrm{m}(\mathrm{H}^+)$ is the activity coefficient of $\mathrm{H}^+(\mathrm{aq})$ (molality basis) at molality $m(\mathrm{H}^+)$, and $m^\ominus = 1\ \mathrm{mol\,kg^{-1}}$ is the standard molality.

Notes:

1. pH cannot be measured independently because calculation of the activity involves the activity coefficient of a single ion. Thus it can be regarded only as a notional definition.
2. The establishment of primary pH standards requires the application of the concept of 'primary method of measurement', assuring full traceability of the results of all measurements and their uncertainties. Any limitation in the theory of determination of experimental variables must be included in the estimated uncertainty of the method.
3. The primary method for measurement of pH involves the use of a cell without transference, known as the Harned cell:

   Pt(s) | H_2(g) | Buffer S, Cl^-(aq) | AgCl(s) | Ag(s)

   The equation for this cell can be rearranged to give:

   $$-\lg[a(\mathrm{H}^+)\,\gamma(\mathrm{Cl}^-)] = \frac{E - E^\ominus}{(R\,T\ln 10)\,/\,F} + \lg[m(\mathrm{Cl}^-)\,/\,m^\ominus]$$

   where E is the potential difference of the cell and $E^\ominus$ is the known standard potential of the AgCl | Ag electrode. Measurements of $E^\ominus$ as a function of $m(\mathrm{Cl}^-)$ are made and the quantity $a(\mathrm{H}^+)\,\gamma(\mathrm{Cl}^-)$ (called the acidity function) is found by extrapolation to $m(\mathrm{Cl}^-)\,/\,m^\ominus = 0$. The value of $\gamma(\mathrm{Cl}^-)$ is calculated using the Bates–Guggenheim convention based on Debye–Hückel theory. Then $\lg[a(\mathrm{H}^+)]$ is calculated and identified as $\mathrm{pH(PS)}$, where PS signifies primary standard. The uncertainties in the two estimates are typically 0.001 in $\lg[a(\mathrm{H}^+)\,\gamma(\mathrm{Cl}^-)]$ and 0.003 in pH. Materials for primary standard buffers must also meet the appropriate requirements for reference materials, including chemical purity and stability, and applicability of the Bates–Guggenheim convention for the estimation of $-\lg[\gamma(\mathrm{Cl}^-)]$ This convention requires that the ionic strength be $\leq 0.1\ \mathrm{mol\,kg^{-1}}$. Primary standard buffers should also lead to small liquid junction potentials when used in cells with liquid junctions. Secondary standards, $\mathrm{pH(SS)}$, are also available, but carry a greater uncertainty in measured values.
4. Practical pH measurements generally use cells with liquid junctions in which, consequently, liquid junction potentials, E_j, are present. Measurements of pH are not normally performed using the Pt|H_2 electrode, but rather the glass (or other H^+ - selective) electrode, whose response factor ($\mathrm{d}E\,/\,\mathrm{dpH}$) usually deviates from the Nernst slope. The associated uncertainties are significantly larger than those associated with fundamental measurements using the Harned cell. Nonetheless, incorporation of the uncertainties for the primary method, and for all subsequent measurements, permits the uncertainties for all procedures to be linked to the primary standards by an unbroken chain of comparisons.
5. Reference values for standards in D_2O and aqueous-organic solvent mixtures exist.

Source:
Green Book, 3rd ed., p. 75
PAC, 1997, *69*, 1007 *(Reference value standards and primary standards for pH measurements in D2O and aqueousorganic solvent mixtures: New accessions and assessments (Technical Report))* on page 1007
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 986

See also:
PAC, 2002, *74*, 2169 *(Measurement of pH. Definition, standards, and procedures (IUPAC Recommendations 2002))* on page 2169
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2205
PAC, 1984, *56*, 567 *(Physicochemical quantities and units in clinical chemistry with special emphasis on activities and activity coefficients (Recommendations 1983))* on page 569

pH glass electrode

A hydrogen-ion responsive electrode usually consisting of a bulb, or other suitable form, of special glass attached to a stem of high resistance glass complete with internal reference electrode and internal filling solution system. Other geometrical forms may be appropriate for special applications, e.g. capillary electrode for measurement of blood pH.

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 540

pH gradient

in electrophoresis

The differential change of pH with distance $(\frac{\mathrm{dpH}}{\mathrm{d}I})$.

Source:
PAC, 1994, *66*, 891 *(Quantities and units for electrophoresis in the clinical laboratory (IUPAC Recommendations 1994))* on page 895

pH standard

See: operational pH standard, primary pH standard, reference value pH standard

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 540

pH-rate profile

A plot of observed rate coefficient, or more usually its decadic logarithm, against pH of solution, other variables being kept constant.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1150

$pH_{0.5}$ or $pH_{1/2}$

in solvent extraction

That value of pH in an aqueous phase at which the distribution ratio is unity at equilibrium. 50% of the solute is extracted ($E = 0.5$) only when the phase ratio is unity.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2385

phantom chain behaviour

Hypothetical behaviour in which chains can move freely through one another when a network is deformed.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1820

pharmacodynamics

Study of pharmacological actions on living systems, including the reactions with and binding to cell constituents, and the biochemical and physiological consequences of these actions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2081

pharmacokinetics

1. Process of the uptake of drugs by the body, the biotransformation they undergo, the distribution of the drugs and their metabolites in the tissues, and the elimination of the drugs and their metabolites from the body over a period of time.
2. Study of such processes.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1064
This definition replaces an earlier definition of pharmacokinetics.

phase

An entity of a material system which is uniform in chemical composition and physical state.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

phase domain

Region of a material that is uniform in chemical composition and physical state.
Notes:

1. A phase in a multiphase material can form domains differing in size.
2. The term 'domain' may be qualified by the adjective microscopic or nanoscopic or the prefix micro- or nano- according to the size of the linear dimensions of the domain.
3. The prefixes micro-, and nano- are frequently incorrectly used to qualify the term 'phase' instead of the term 'domain'; hence, 'microphase domain', and 'nanophase domain' are often used. The correct terminology that should be used is phase microdomain and phase nanodomain.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2001

phase fluorimetry

See: lifetime of luminescence

Source:
Orange Book, p. 197

phase I reaction

of biotransformation

Enzymic modification of a substance by oxidation, reduction, hydrolysis, hydration, dehydrochlorination, or other reactions catalyzed by enzymes of the cytosol, of the endoplasmic reticulum (microsomal enzymes) or of other cell organelles.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1064

phase II reaction

of biotransformation

Binding of a substance, or its metabolites from a phase I reaction, with endogenous molecules (conjugation), making more water-soluble derivatives that may be excreted in the urine or bile.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1064

phase interaction

Molecular interaction between the components present in the interphases of a multiphase mixture.
Note:
The interphase elasticity is the capability of a deformed interphase to return to its original dimensions after the force causing the deformation has been removed.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2002

phase inversion

A term used in two senses which should be specified: density inversion or continuity inversion.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2387

phase ratio, β

in chromatography

The ratio of the volume of the mobile phase to that of the stationary phase in a column:

$$\beta = \frac{V_0}{V_s}$$

In the case of open-tubular columns the geometric internal volume of the tube (V_c) is to be substituted for V_0.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 833
Orange Book, p. 100

phase ratio, r

in liquid-liquid distribution

The ratio of the quantity of the solvent to that of the other phase.
Notes:

1. Unless otherwise specified the phase ratio refers to the phase volume ratio.
2. If other aspects of the phase ratio are employed viz. phase mass ratio, phase flow ratio, these should be specified.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2385

phase rule

The number of degrees of freedom, F, that a system containing C components can have when P phases are in equilibrium, is given as:

$$F = C - P + 2$$

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

phase separation

The process by which a single solid (liquid) phase separates into two or more new phases.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

phase transition

A change in the nature of a phase or in the number of phases as a result of some variation in externally imposed conditions, such as temperature, pressure, activity of a component or a magnetic, electric or stress field.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

phase-space theory

This is a theory applied to unimolecular or bimolecular reactions proceeding through long-lived complexes. The probability of reaction is assumed to be proportional to the number of states available to a particular product channel divided by the number of states corresponding to all product channels. The theory is used to predict rates, product energy distributions, product velocity distributions, and product angular momentum distributions.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 176

phase-transfer catalysis

The phenomenon of rate enhancement of a reaction between chemical species located in different phases (immiscible liquids or solid and liquid) by addition of a small quantity of an agent (called the 'phase-transfer catalyst') that extracts one of the reactants, most commonly an anion, across the interface into the other phase so that reaction can proceed. These catalysts are salts of 'onium ions' (e.g. tetraalkylammonium salts) or agents that complex inorganic cations (e.g. crown ethers). The catalyst cation is not consumed in the reaction although an anion exchange does occur.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1150

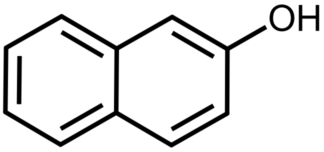
phenolates

Synonymous with phenoxides. The term phenolate should not be used for solvates derived from a phenol, for the ending -ate often occurs in names for anions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357

phenols

Compounds having one or more hydroxy groups attached to a benzene or other arene ring, e.g. 2-naphthol:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357

phenomenological equation

In the following only media which are isotropic with respect to mass transport (i.e. the transport coefficients are independent of direction) are being considered. In the linear range (not too far from equilibrium), for uniform temperature and neglecting external fields such as the earth's gravitational field, the flux density of species B is related to the gradients of the electrochemical potentials of all species by the phenomenological equation:

$$N_{\mathrm{B}} - c_{\mathrm{B}}\, v_{\mathrm{A}} = -\sum_{\substack{i \\ i \neq A}} L_{\mathrm{B}\,i}^{\mathrm{A}}\, \nabla \mu_i$$

with

$$i = \mathrm{B}, \mathrm{C}, \ldots$$

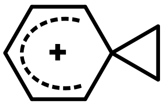
where $\nabla \mu_i$ is the gradient of the electrochemical potential of species i. The proportionality factors $L^{\mathrm{A}}_{\mathrm{B}i}$ are called phenomenological coefficients. Their values depend on the frame of reference. The latter is taken here to move with the velocity v_{A} of species A, and hence:

$$L^{\mathrm{A}}_{\mathrm{A}i} = 0.$$

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1830

phenonium ions

The traditional generic name for those cyclohexadienyl cations that are spiro-annulated with a cyclopropane unit. Phenonium ions constitute a subclass of arenium ions.



See also: bridged carbocation

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357

phenotype

The observable structural and functional characteristics of an organism determined by its genotype and modulated by its environment.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

phenoxides

Salts or analogous metal derivatives of phenols; synonymous with phenolates. A preferable general term, however, is aryloxides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357

pheromone

Synonyms: ectohormone, feromone

Substance used in olfactory communication between organisms of the same species eliciting a change in sexual or social behaviour. Synonymous with ectohormone, feromone.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2082

phonon

Elementary excitation in the quantum mechanical treatment of vibrations in a crystal lattice. An energy bundle that behaves as a particle of energy $h\nu$, with ν the vibration frequency and h the Planck constant.
Notes:

1. A phonon can be considered as an acoustic mode of thermal vibration of a crystal lattice (or liquid helium II).
2. Every harmonic vibration can be decomposed in phonons, which are the elementary vibrations. The total number of phonons in a system that has internal vibrations (e.g., a crystal) is related to the temperature of the system.
3. The concept of phonons provides a simplification in the theories of thermal and electrical conduction in solids.
4. For example, interactions between phonons and electrons are thought to be responsible for such phenomena as 'superconductivity'.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 382

phosphanes

The saturated hydrides of tervalent phosphorus having the general formula P_nH_{n+2} . Individual members having an unbranched phosphorus chain are named phosphane, diphosphane, triphosphane, etc. The name of a saturated hydride of phosphorus wherein one or more phosphorus atoms have a bonding number of 5 is formed by prefixing locants and λ^5 symbols to the name of the corresponding phosphane. Hydrocarbyl derivatives of PH_3 belong to the class phosphines.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357

phosphanylidenes

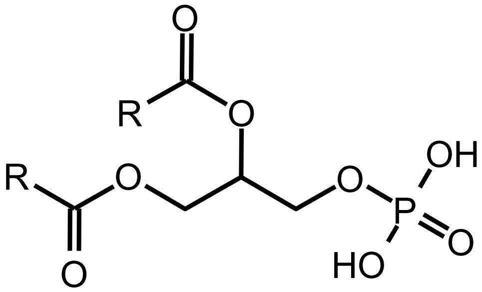
Synonym: phosphinidenes

Recommended name for carbene analogues having the structure RP: (former IUPAC name is phosphinediyls). A common non-IUPAC synonym is phosphinidenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357

phosphatidic acids

Derivatives of glycerol in which one hydroxy group, commonly but not necessarily primary, is esterified with phosphoric acid and the other two are esterified with fatty acids.

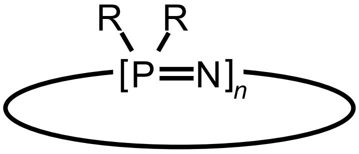


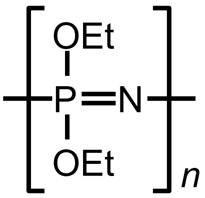
See: lecithins, phosphoglycerides, phospholipids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357
White Book, p. 184

phosphazenes

Compounds containing a phosphorus–nitrogen double bond, i.e. derivatives of $H_3P=NH$ and $HP=NH$. A multiplicity of such bonds is present in various well-established chain, ring and cage compounds. E.g.





poly(diethoxyphosphazene)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357

phosphine oxides

Compounds having the structure $R_3P{=}O \longleftrightarrow R_3P^+{-}O^-$ (analogously, phosphine imides and phosphine sulfides).
See: imides (2)

Source:
PAC, 1995, *67*, 1533 *(Use of immunoassays for the analysis of pesticides and some other organics in water samples (Technical Report))* on page 1537

phosphines

PH_3 and compounds derived from it by substituting one, two or three hydrogen atoms by hydrocarbyl groups R_3P . RPH_2 , R_2PH and R_3P ($R \neq H$) are called primary, secondary and tertiary phosphines, respectively. A specific phosphine is preferably named as a substituted phosphane, e.g. CH_3PH_2 methylphosphane.
See: phosphanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357

phosphinic acids

$H_2P(=O)OH$ (phosphinic acid) and its P-hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1357

phosphinous acids

H_2POH (phosphinous acid) and its P-hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phospho

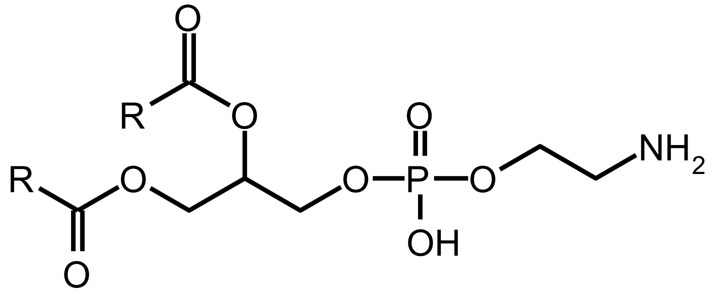
1. A prefix used in biochemical nomenclature in place of phosphono to denote the $-P(=O)(OH)_2$ group linked to a heteroatom, e.g. $Me_3N^+{-}CH_2CH_2{-}OP(=O)(OH)O^-$ phosphocholine.
2. An infix used in biochemical nomenclature to name phosphoric diesters, e.g. glycerophosphocholine.

See: phosphoglycerides

Source:
White Book, p. 256
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phosphoglycerides

Phosphoric diesters, esters of phosphatidic acids, generally having a polar head group (OH or NH_2) on the esterified alcohol which typically is 2-aminoethanol, choline, glycerol, inositol, serine. The term includes lecithins, cephalins. E.g.



2-aminoethyl phosphatidates

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phospholipids

Lipids containing phosphoric acid as mono- or di-esters, including phosphatidic acids and phosphoglycerides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

See also:
White Book, p. 184

phosphonic acids

$HP(=O)(OH)_2$ (phosphonic acid) and its P-hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phosphonitriles

Compounds of stoichiometric composition $[X_2PN]_n$, in which X is alkoxy, halogen, or other electronegative group, and n is a variable integer, the value of which may not be known.
See: phosphazenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phosphonium compounds

Salts (and hydroxides) $[R_4P^+]X^-$ containing tetracoordinate phosphonium ion and the associated anion.
See: onium compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phosphonium ylides

Synonyms: phosphorus ylides, Wittig reagents

Compounds having the structure $R_3P^+–C^-R_2 \longleftrightarrow R_3P=CR_2$. Also known as Wittig reagents.
See: ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phosphono

A prefix indicating the presence of the group $–P(=O)(OH)_2$.
See: phospho

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phosphonous acids

$HP(OH)_2$ (phosphonous acid) and its P-hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phosphoramides

Compounds in which one or more of the OH groups of phosphoric acid have been replaced with an amino or substituted amino group; commonly confined to the phosphoric triamides, $P(=O)(NR_2)_3$, since replacement of one or two OH groups produces phosphoramidic acids $P(=O)(OH)(NR_2)_2$, $P(=O)(OH)_2(NR_2)$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phosphoranes

The mononuclear hydride PH_5 , systematically named λ^5-phosphane, and its hydrocarbyl derivatives. By extension, the literature also applies the term to phosphonium ylides.
See also: phosphanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1358

phosphoranyl radicals

A tetracoordinate phosphorus species which has nine valence-shell electrons $R_4P^{\cdot}$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

phosphorescence

From a phenomenological point of view, the term has been used to describe long-lived luminescence. In mechanistic photochemistry, the term designates luminescence involving change in spin multiplicity, typically from triplet to singlet or vice versa. The luminescence from a quartet state to a doublet state is also phosphorescence.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2258
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 233

See also:
Orange Book, p. 184

phosphorescence lifetime

Parameter describing the time evolution of the decay of the phosphorescence radiant intensity.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 383

phosphoroscope

A mechanical device used to separate phosphorescence from fluorescence.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 238

phosphorylation

A process (catalysed by enzymes) involving the transfer of a phosphate group from a donor to a suitable acceptor; in general, an ester linkage is formed, for example:
ATP + alcohol$\longrightarrow$ADP + phosphate ester

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1291

phosphylenes [obsolete]

An obsolescent synonym for phosphanylidenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

photo-Bergman cyclization

Intramolecular photoinduced cyclization of enediynes leading to aromatic compounds.
Notes:

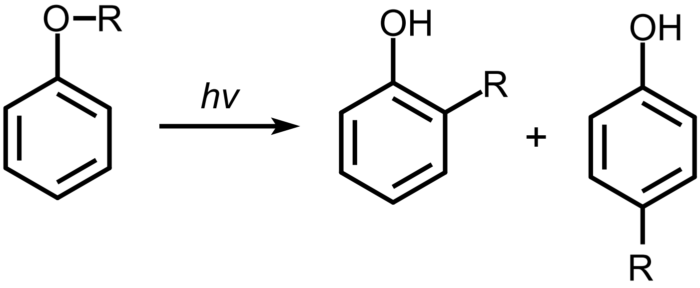
1. The solvent plays a key role in the reaction efficiency and product distribution. The reversibility of the initial photoreaction and competing radical *vs* ionic pathways dictate product distribution, in stark contrast to the thermal process.
2. This reaction is particularly attractive in molecular biology and molecular medicine. In particular, it permits the expeditious synthesis of core synthones of great diversity.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 384

photo-Claisen rearrangement

Rearrangement closely related to the photo-Fries rearrangement; it is experienced by aryl ethers (instead of aryl esters) and follows an analogous mechanism.

Note:
An example is the photoinduced rearrangement of phenyl ethers to *ortho* and *para*-alkyl phenols.



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 387

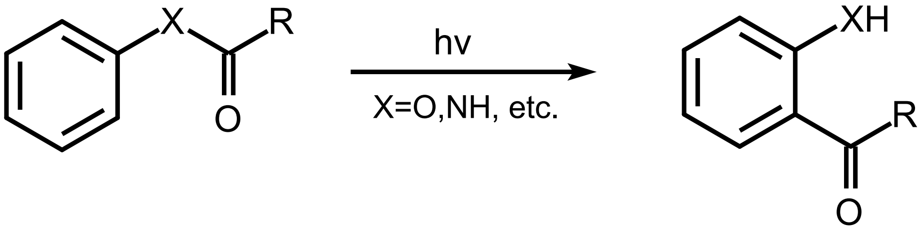
photo-elastic polymer

Polymer that, under stress, exhibits birefringence.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 901

photo-Fries rearrangement

A photorearrangement of aryl or acyl esters to give the [1,3]-rearranged product (as well as the [1,5]-rearranged product):



Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2261

photoacoustic detector

A pressure-sensitive detector used to detect intermittent radiation absorbed in a black body or in the sample concerned. The resulting rapid temperature change produces a transient pressure oscillation that is observed with the help of a microphone, or a piezoelectric device.
See also: radiation detector

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1752

photoacoustic effect

Generation of heat after absorption of radiation, due to radiationless deactivation or chemical reaction.
See also: photoacoustic spectroscopy

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2258

photoacoustic spectroscopy

A spectroscopic technique based on the photoacoustic effect. A photoacoustic spectrum consists of a plot of the intensity of the acoustic signal detected by a microphone or a 'piezoelectric' detector, against the excitation wavelength or another quantity related to the photon energy of the modulated excitation.
See also: isooptoacoustic point

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2259

photoadsorption

Also contains definition of: photodesorption

Irradiation by light (usually visible or ultraviolet) may affect adsorption. In a system containing adsorptive and adsorbent exposure to light may lead to increased adsorption (photoadsorption) or it may lead to desorption of an adsorbate (photodesorption).

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 77

photoaffinity labelling

Acronym: PAL

Technique by which a photochemically reactive molecular entity, specifically associated with a biomolecule, is photo-excited in order to covalently attach a label to the biomolecule, usually via intermediates. Identification of the resulting photo-crosslinked product provides structural information on the protein′s binding site.
Notes:

1. Technique widely used for identifying in general ligand-receptor interactions in biological macromolecules and in particular the binding site within proteins.

2. Typical examples are nitrenes, carbenes, ketone excited states, cations and radicals.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 383

photoassisted catalysis

Catalytic reaction involving production of a catalyst by absorption of light.
See: photocatalysis

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2259

photobiology

Branch of biology concerned with the biological and bioenvironmental effects of ultraviolet, visible or infrared radiation.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 384

photocatalysis

Change in the rate of a chemical reaction or its initiation under the action of ultraviolet, visible or infrared radiation in the presence of a substance—the photocatalyst—that absorbs light and is involved in the chemical transformation of the reaction partners.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 384

photocatalyst

Catalyst able to produce, upon absorption of light, chemical transformations of the reaction partners. The excited state of the photocatalyst repeatedly interacts with the reaction partners forming reaction intermediates and regenerates itself after each cycle of such interactions.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 384

photochemical curing

Also contains definition of: photo-curing

Curing induced by photo-irradiation.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1822

photochemical equivalence

According to the principle of photochemical equivalence, there is a one-to-one relationship between the number of photons absorbed by a system and the number of excited species produced. The principle often fails for light of high intensity (e.g. laser beams), when molecules may absorb more than one photon.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 176

photochemical funnel

Molecular structure where the excited-state reactant or intermediate is delivered to the ground state to initiate product formation.
Note:
For a broad class of organic reactions, the structure of the funnel can take the form of a conical intersection or a singlet–triplet crossing.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 385

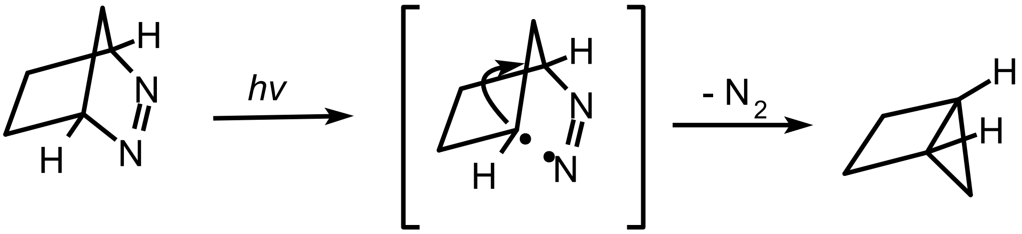
photochemical hole burning

See: hole burning

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2259

photochemical nitrogen extrusion

Photoinduced dinitrogen (N_2) elimination.
Note:
Typical examples are the photoinduced denitrogenation of azoalkanes. The following scheme also show the diazenyl radical intermediate.



diazenyl biradical

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 385

photochemical reaction

Synonym: photoreaction

Generally used to describe a chemical reaction caused by absorption of ultraviolet, visible or infrared radiation. There are many ground-state reactions, which have photochemical counterparts. Among these are photochemical nitrogen extrusions, photocycloadditions, photodecarbonylations, photodecarboxylations, photoenolizations, photo-Fries rearrangement, photoisomerizations, photooxidations, photorearrangements, photoreductions, photosubstitutions, etc.
Note:
Photochemical paths offer the advantage over thermal methods of forming thermodynamically disfavoured products, overcome large activation barriers in a short period of time, and allow reactivity otherwise inaccessible by thermal methods.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 386

photochemical reaction path

Sequence of geometries adopted by a molecule after initial electronic excitation, combined with a specification of the electronic state at each geometry, from radiation absorption to product formation. Theoretically, this usually involves the computation of the MERP connecting the Franck–Condon point, located on the potential-energy surface of the spectroscopic state, to the final photoproducts located on the ground-state potential ?energy surface. Experimentally, a photochemical reaction path can be probed by detecting transient species or reaction intermediates.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 386

photochemical smog

Product of photochemical reactions caused by solar radiation and occurring in polluted air as well as in air contaminated by compounds emitted by natural sources, such as those emitted by vegetation.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 386

photochemical yield

See: quantum yield

Source:
Green Book, 2nd ed., p. 57

photochemistry

The branch of chemistry concerned with the chemical effects of light (far UV to IR).
See: photochemical reaction

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2259

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2206

photochromism

Reversible transformation of a molecular entity between two forms, A and B, having different absorption spectra, induced in one or both directions by absorption of electromagnetic radiation. The spectral change produced is typically, but not necessarily, of visible colour and is accompanied by differences in other physical properties.
The thermodynamically stable form A is transformed by irradiation into form B. The back reaction can occur thermally (photochromism of type T) or photochemically (photochromism of type P).

$$\mathbf{A} \xrightleftharpoons[h\nu_2 \text{or } \Delta]{h\nu_1} \mathbf{B}$$

The terms 'switch-on' and 'switch-of' are sometimes used to denote the two directions of the photochromic reaction.
Note:
An important parameter is the 'number of cycles' that a photochromic system can undergo under well-defined conditions (solution, matrix, concentration, temperature).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 387

photoconductive detector

In a photoconductive detector an electric potential is applied across the absorbing region and causes a current to flow in proportion to the irradiance if the photon energy exceeds the energy gap between the valence and the conduction band. Depending on their spectral responsivity function, photoconductive detectors are divided into photoconductive detectors for the visible wavelength range e.g. cadmium sulfide or CdS photoconductive detectors, photoconductive detectors for the near infrared wavelength range e.g. lead sulfide or PbS photoconductive detectors, photoconductive detectors for the infrared wavelength range e.g. silicon doped with arsenide or Si:As photoconductive detectors, and the mercury-cadmium-telluride or HgCdTe photoconductive detector.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1754

photoconductivity

Electrical conductivity resulting from photoproduction of charge carriers.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2259

photocrosslinking

The formation of a covalent linkage between two macromolecules or between two different parts of one macromolecule.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2260

photocurrent yield

The quantum efficiency of electron transport between the two electrodes of a photovoltaic cell or photoelectrochemical cell.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2260

photocyclization

Intramolecular photochemical process leading to carbo- or hetero- cyclic ring systems by formation of one new single bond, either by a concerted process (e.g., electrocyclization) or by multi-step processes such as Norrish–Yang reaction, photoinduced electron transfer processes, Yang photocyclization and others.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 388

photocycloaddition

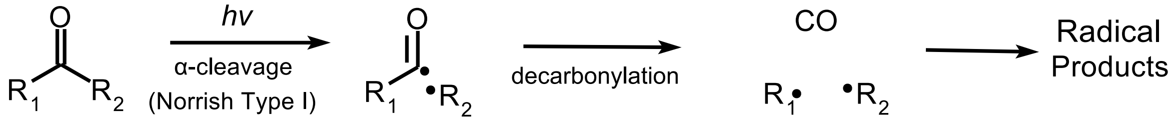
Intermolecular photochemical process leading to carbo- or hetero- cyclic ring systems by formation of two new single bonds, either by a concerted process (e.g., a concerted addition) or by multi-step processes (e.g., the Paternò–Büchi reaction).
Note:
Triplet state photocycloadditions are two-step processes involving the formation of diradical intermediates.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 388

photodecarbonylation

Photoinduced extrusion of carbon monoxide (CO).
Notes:

1. Typical example is the Norrish Type I photoreaction, in which, after production of the diradical upon photoinduced α-cleavage, CO is eliminated. This reaction has been widely exploited for the production of radicals in crystals, as well as for the synthesis of cyclic compounds.

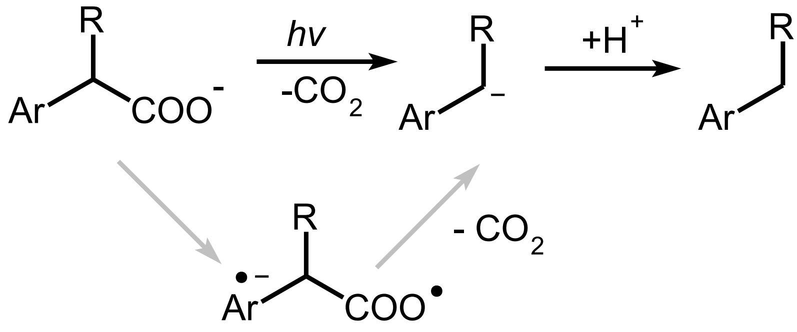


2. Another example is the photodecarbonylation of alpha-aryl aldehydes.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 388

photodecarboxylation

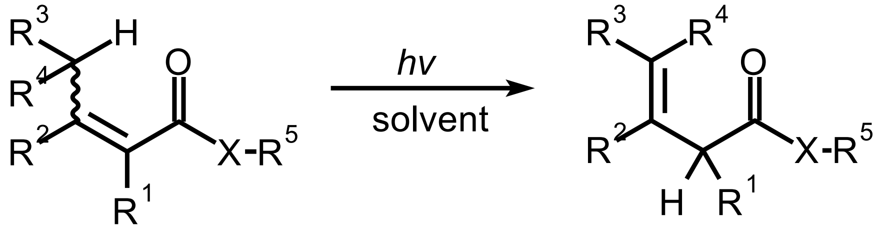
Photoinduced extrusion of carbon dioxide (CO_2).
Note:
Typical examples are the CO_2 extrusion upon excitation of anti-inflamatory 2-arylpropionic acids, such as ketoprofen.



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 389

photodeconjugation

Photoinduced reaction of conjugated compounds (e.g., enones and carboxylic acid derivatives) leading to loss of conjugation.



X= O, NH

Note:
This reaction has important synthetic applications for the synthesis of frameworks of numerous natural products, such as β,γ-unsaturated carboxylic acids from photoexcitation of α,β-unsaturated carboxylic acid derivatives, excluding the use of strong bases, as required for similar isomerizations performed in the ground state.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 389

photodegradation

The photochemical transformation of a molecule into lower molecular weight fragments, usually in an oxidation process. This term is widely used in the destruction (oxidation) of pollutants by UV-based processes.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2260

photodetachment

of electrons

Ejection of an electron from a negative ion upon photoexcitation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2260

photodiode

Also contains definitions of: avalanche photodiode, PIN (p-intrinsic-n) diode, Schottky-barrier photodiode

A two-electrode, radiation-sensitive junction formed in a semiconductive material. A junction is formed by two successive regions of a semiconductive material having, respectively, an excess of electrons (n-type) or holes (p-type). A bias potential applied to the detector creates a region at the interface that is depleted of majority carriers. Each incident photon produces electron-hole pairs in the depletion region resulting in a measurable signal current. The photodiode can be operated either with zero bias in the photovoltaic mode where the photodiode is actually generating the electric potential supplied to the load. In a biased mode, the photoconductive mode, the reverse current is proportional to the irradiation. A Schottky-barrier photodiode is constructed by deposition of a metal film on a semiconductor surface in such a way that no interface layer is present. The barrier thickness depends on the impurity dopant concentration in the semiconductor layer. The incident radiation generates electon-hole pairs within the depletion region of the barrier where they are collected efficiently and rapidly by the built-in field. A PIN (p-intrinsic-n) diode is a planar diffused diode consisting of a single crystal having an intrinsic (undoped or compensated) region sandwiched between p- and n-type regions. A bias potential applied across the detector depletes the intrinsic region of charge carriers, constituting the radiation-sensitive detector volume. The number of electron-hole pairs produced is dependent on the energy of the incident photons. An avalanche photodiode is a photodiode in which the photogenerated electron-hole pairs are accelerated by a bias potential near to breakdown potential so that further electron-hole pairs are formed leading to saturation of the photocurrent. This operational mode for photon counting is the so-called Geiger mode, similar to that of the gas filled Geiger counter. Avalanche photodiodes can also be operated in the proportional mode.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1755

photodiode array

An arrangement of a number of photodiodes on a single chip.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1756

photodynamic effect

A term used in photobiology to refer to photoinduced damage requiring the simultaneous presence of light, photosensitizer and molecular oxygen. A sensitized photooxidation which involves molecular oxygen.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2260

photoelectric attenuation coefficient

The attenuation coefficient when only the photoelectric process is taken into account.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

photoelectric peak

Synonym: photopeak

Of a spectrum of γ-radiation, the part of the spectral response curve corresponding to the absorption in the radiation detector by the photoelectrical effect of the detected γ-energy. In most cases the peak also contains events caused by multiple processes and use of the expression total absorption peak or full energy peak is to be preferred. Synonymous with photopeak.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

photoelectrical effect

The ejection of an electron from a solid or a liquid by a photon.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2260
Orange Book, p. 234

photoelectrochemical cell

An electrochemical cell in which current and a voltage are simultaneously produced upon absorption of light by one or more of the electrodes. Usually at least one of the electrodes is a semiconductor.
See also: photovoltaic cell, photoelectrolytic cell, photogalvanic cell

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2260

PAC, 1991, *63*, 569 *(Terminology in semiconductor electrochemistry and photoelectrochemical energy conversion (Recommendations 1991))* on page 593

photoelectrochemical etching

The dissolution of a semiconductor in an electrolytic solution upon exposure to light. Used in the photopatterning of semiconductor surfaces.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2260

photoelectrochemistry

A term applied to a hybrid field of chemistry employing techniques which combine photochemical and electrochemical methods for the study of the oxidation-reduction chemistry of the ground or excited states of molecules or ions. In general, it is the chemistry resulting from the interaction of light with electrochemical systems.
See also: photoelectrochemical cell, photogalvanic cell, photovoltaic cell

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2260

photoelectrolytic cell

Also contains definition of: photocatalytic cell

A cell in which radiant energy causes a net chemical conversion in the cell, e.g. so as to produce hydrogen as a useful fuel. These cells can be classified as photosynthetic or photocatalytic. In the former case, radiant energy provides a Gibbs energy to drive a reaction such as $H_2O \rightarrow H_2 + \frac{1}{2}O_2$, and electrical or thermal energy may be later recovered by allowing the reverse, spontaneous reaction to proceed. In a photocatalytic cell the photon absorption promotes a reaction with $\Delta G < 0$ so there is no net storage of chemical energy, but the radiant energy speeds up a slow reaction.

Source:
PAC, 1991, *63*, 569 *(Terminology in semiconductor electrochemistry and photoelectrochemical energy conversion (Recommendations 1991))* on page 593

See also:
PAC, 1991, *63*, 569 *(Terminology in semiconductor electrochemistry and photoelectrochemical energy conversion (Recommendations 1991))* on page 596

photoelectron spectroscopy (PES)

Also contains definitions of: ESCA, XPS

A spectroscopic technique which measures the kinetic energy of electrons emitted upon the ionization of a substance by high energy monochromatic photons. A photoelectron spectrum is a plot of the number of electrons emitted versus their kinetic energy. The spectrum consists of bands due to transitions from the ground state of an atom or molecular entity to the ground and excited states of the corresponding radical cation. Approximate interpretations are usually based on 'Koopmans theorem' and yield orbital energies. PES and UPS (UV photoelectron spectroscopy) refer to the spectroscopy using vacuum ultraviolet sources, while ESCA (electron spectroscopy for chemical analysis) and XPS use X-ray sources.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2261
PAC, 1976, *45*, 221 *(Nomenclature and Spectral Presentation in Electron Spectroscopy Resulting from Excitation by Photons)* on page 223
Orange Book, p. 246

photoelectron yield

The number of photoelectrons emitted by the sample per incident photon.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

photoemissive detector

Also contains definition of: external photoelectric effect

A detector in which a photon interacts with a solid surface, which is called the photocathode, or a gas, releasing a photoelectron. This process is called the external photoelectric effect. The photoelectrons are collected by an electrode at positive electric potential, i.e. the anode.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1752

photoexcitation

The production of an excited state by the absorption of ultraviolet, visible, or infrared radiation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2261

photogalvanic cell

An electrochemical cell in which current or voltage changes result from photochemically generated changes in the relative concentrations of reactants in a solution phase oxidation-reduction couple.
See also: photovoltaic cell

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2261

See also:
PAC, 1991, *63*, 569 *(Terminology in semiconductor electrochemistry and photoelectrochemical energy conversion (Recommendations 1991))* on page 596

photohydration

Photochemical process leading to the addition of water across a C–C double (or triple) bond or to a carbonyl (or carbonyl analogue) group.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 392

photoinduced electron transfer

An electron transfer resulting from an electronic state produced by the resonant interaction of electromagnetic radiation with matter.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2261

photoinduced polymerization

The polymerization of a monomer by a free radical or ionic chain reaction initiated by photoexcitation.
See: photoinitiation

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2261

photoinitiation

The photoproduction of a free radical or ion capable of initiating a chain reaction such as a polymerization.
See: photoinduced polymerization

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2261

photoionization

The term generally used to describe ionization of any species by photons. The process may, for example, be written

$$\mathrm{M} + h\nu \longrightarrow \mathrm{M}^{+\bullet} + \mathrm{e}$$

Electrons and photons do not 'impact' molecules or atoms; they interact with them in ways that result in various electronic excitations including ionization. For this reason it is recommended that in mass spectrometry the terms 'electron impact' and 'photon impact' not be used.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2261
Orange Book, p. 203

photoionization detector

in gas chromatography

Radiation from an ultraviolet lamp ionizes certain species in the carrier gas. A potential difference is applied and the resulting ionization current is detected. The detector is only useful for substances with ionization potentials below about $11\ \mathrm{eV}$. This makes it quite useful for detecting one component of a combined eluent when the other component, for instance nitrogen, has a high ionization potential. The detector has a small linear dynamic range and is capable of detecting substances below $1\ \mathrm{ppmv}$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2191

photoisomerization

Photochemical process leading to an isomerization of the substrate, either by bond rotation, skeletal rearrangement or atom- or group- transfer.
Notes:

1. Typical examples are *cis-trans* photosomerization of alkenes, polyenes and phototautomerization.
2. Photochemical pathways have the advantage over thermal and catalytic methods of giving isomer mixtures (photostationary states) rich in thermodynamically unstable isomers.
3. Photoisomerization is the primary photochemical reaction of the chromophore in several biological photoreceptors such as retinal proteins (e.g., rhodopsin), phytochromes, and the photoactive yellow protein.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 393

photoluminescence

Luminescence from direct photoexcitation the emitting species.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 393

photoluminescent polymer

Polymer that exhibits luminescence (i.e., fluorescence or phosphorescence arising from photo-excitation).
See: photoluminescence.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 901

photolysis

The cleavage of one or more covalent bonds in a molecular entity resulting from absorption of light, or a photochemical process in which such cleavage is an essential part. For example:

$$\mathrm{Cl_2} \longrightarrow 2\,\mathrm{Cl}^{\bullet}$$

The term is used incorrectly to describe irradiation of a sample, although in the combination flash photolysis this usage is accepted.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1150

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2206

photometry

The measurement of light over wavelengths which produce visual sensation (approximately 380 - 780 nm). Thus photometric quantities do not refer to a specific wavelength but to the light emitted by a standard source (formerly a 'standard international candle', now a blackbody radiator emitting at the temperature of solidifying platinum, 2042 K). Luminance and illuminance are the photometric analogues of the radiometric quantities radiance and irradiance, respectively, but conversion from photometric units (e.g. $\mathrm{lm\,cm^{-2}}$) to radiometric units (e.g. $\mathrm{J\,s^{-1}\,cm^{-2}}$) requires convolution over wavelength of the spectral radiation with the relative spectral response of the human eye. The standard response is called the 'spectral luminous efficiency of radiation', and is tabulated for daylight adapted vision in photopic response tables.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2206

photomultiplier tube

Also contains definitions of: channel photomultiplier tube, strip dynode photomultiplier tube

A vacuum phototube with additional amplification by electron multiplication. It consists of a photocathode, a series of dynodes, called a dynode chain on which a secondary-electron multiplication process occurs, and an anode. According to the desired response time, transit time, time spread, gain, or low dark current, different types of dynode structures have been developed, e.g. circular cage structure, linear focused structure, venetian blind structure, box and grid structure. Some special dynode structures permit combination with additional electric or magnetic fields. A strip dynode photomultiplier tube consists of a photocathode followed by thin dynode material on an insulating substrate. In a continuous-strip photomultiplier, two strip dynodes are arranged in parallel. A potential applied to the ends of the two strips produces an electric field across the continuous strip dynodes, giving rise to electron multiplication along the dynodes. In a resistance-strip magnetic photomultiplier, a uniform magnetic field is applied to the planes of the strips, so that the electrons travel in the crossed electric and magnetic fields. A channel photomultiplier tube photocathode consists of a channel electron multiplier (CEM) system for the photoelectrons, and an anode to collect the final electron current. The basic part of the CEM is a tube with a semiconducting inner surface. In general it is curved in order to inhibit the acceleration of positive ions towards the photocathode. A number of small channels called microchannels can be constructed in arrays for imaging applications.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1753

See also:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

photon

Particle of zero charge, zero rest mass, spin quantum number 1, energy $h\,\nu$ and momentum $\frac{h\,\nu}{c}$ (h is the Planck constant, ν the frequency of radiation and c the speed of light), carrier of electromagnetic force.

Source:
Green Book, 2nd ed., p. 93

PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2262

photon activation

See: activation *in radiochemistry*

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

photon counting

Also contains definition of: single-photon counting

Recording of sequential single photons counted by way of recording and counting sequential electron pulses at the anode of the photomultiplier.
Notes:

1. Each electron pulse consists of 10^5–10^6 electrons resulting from the multiplication, in the 'dynode' arrangement (or the microchannel plate) of a photomultiplier, of a single photoelectron emitted by a photosensitive layer (the photocathode of the photomultiplier) upon arrival of a single photon.
2. Technique used for two purposes: (i) sensitive measurement of low levels of radiation such as those originating from a luminophore and (ii) recording of emission decays.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 393

photon echo

Time-resolved optical spectroscopy in which the inhomogeneous broadening of absorbers is eliminated by the proper choice of geometry in a four-wave mixing experiment.
Notes:

1. Term applied to a group of non-linear optical techniques such as integrated echo, time-gated echo, three-pulse echo peak shift, heterodyne-detected echo and 2D-echo.
2. Photon echo techniques make use of the third-order optical polarization and 'hyper-susceptibility'. The main distinguishing feature of photon echo methods from all other third-order processes is the time ordering of the field interactions that leads to a rephasing process in the induced polarization to remove inhomogeneous contributions to the absorption linewidth.
3. In terms of mathematical description, the photon echo is equal to the spin echo (solid-state physics) from which a term 'echo' was borrowed.
4. Technique used, e.g., to probe solvation dynamics upon (ultra-short) pulse excitation of a chromophore.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 394

photon exitance, M_p

Also contains definition of: specific photon emission

Synonym: photon emittance

Photon flux, number basis, q_p, emitted by an element of the surface containing the source point under consideration divided by the area S of that element. SI unit is s^{-1} m^{-2}.
Notes:

1. Mathematical definition: $\mathrm{d}q_p / \mathrm{d}S$. If q_p is constant over the surface area considered, $M_p = q_p / S$.
2. Formerly called photon emittance.
3. This quantity can be expressed on a chemical amount basis by dividing M_p by the Avogadro constant. In this case the symbol is $M_{n,p}$, the name 'photon exitance, amount basis', SI unit is mol s^{-1} m^{-2}; common unit is einstein s^{-1} m^{-2}.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 394

photon exposure, H_p

Photon irradiance, E_p, integrated over the time of irradiation for a beam incident from all upward directions. SI unit is m^{-2}.
Notes:

1. Mathematical definition: $H_p = \int_t E_p \mathrm{d}t$. If the photon irradiance is constant over the time interval, $H_p = E_p\, t$.
2. This term refers to a beam not scattered or reflected by the target or its surroundings. For a beam incident from all directions photon fluence ($H_{p,o}$, $F_{p,o}$) is an equivalent term.
3. This quantity can be used on a chemical amount basis by dividing H_p by the Avogadro constant, the symbol then being $H_{n,p}$, the name 'photon exposure, amount basis', SI unit is mol m^{-2}; common unit is einstein m^{-2}.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 394

photon flow, Φ_p

The number of photons (quanta, N) per unit time. ($\frac{\mathrm{d}N}{\mathrm{d}t}$, simplified expression: $\Phi_p = \frac{N}{t}$ when the number of photons is constant over the time considered). The SI unit is s^{-1}. Alternatively, the term can be used with the amount of photons (mol or its equivalent einstein), the SI unit then being mol s^{-1}.

See: spectral photon flow
See also: radiant power

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2263

photon fluence, $H_{\mathrm{p,o}}$, $F_{\mathrm{p,o}}$

Amount of photons (quanta of radiation) incident on a small sphere from all directions, divided by the cross-sectional area of that sphere and integrated over time. Photons per surface area ($\mathrm{quanta\ m^{-2}}$). SI unit is $\mathrm{m^{-2}}$.
Notes:

1. Mathematical definition: $H_{\mathrm{p,o}} = F_{\mathrm{p,o}} = \mathrm{d}N_{\mathrm{p}} / \mathrm{d}S = \int_t E_{\mathrm{p,o}} \mathrm{d}t$ with $E_{\mathrm{p,o}}$ the photon fluence rate, integrated over the duration of the irradiation, t. If $E_{\mathrm{p,o}}$ is constant over the time interval, $H_{\mathrm{p,o}} = F_{\mathrm{p,o}} = E_{\mathrm{p,o}}\, t$
2. This quantity can be used on a chemical amount basis by dividing $H_{\mathrm{p,o}}$ by the Avogadro constant, the symbol then being $H_{n,\mathrm{p,o}}$, the name 'photon fluence, amount basis', SI unit is $\mathrm{mol\ m^{-2}}$; common unit is $\mathrm{einstein\ m^{-2}}$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 395

photon fluence rate, $E_{\mathrm{p,o}}$

Rate of photon fluence. Total number of photons (N_{p}) incident from all directions on a small sphere divided by the cross-sectional area of the sphere and per time interval. SI unit is $\mathrm{m^{-2}\ s^{-1}}$. Same as photon spherical irradiance.
Notes:

1. Mathematical definition: $E_{\mathrm{p,o}} = \mathrm{d}N_{\mathrm{p}} / (\mathrm{d}t\ \mathrm{d}S) = \mathrm{d}H_{\mathrm{p,o}} / \mathrm{d}t$. If $E_{\mathrm{p,o}}$ is constant over the time interval and the surface, $E_{\mathrm{p,o}} = N_{\mathrm{p}} / t\, S$ Equivalent definition: $E_{\mathrm{p,o}} = \int_{4\pi} L_{\mathrm{p}} \mathrm{d}\Omega$ with L_{p} the photon radiance and Ω the solid angle of the beams passing through the given point on the surface.
2. It reduces to photon irradiance E_{p} for a parallel and normally incident beam not scattered or reflected by the target or its surroundings.
3. This quantity can be used on a chemical amount basis by dividing $E_{\mathrm{p,o}}$ by the Avogadro constant, the symbol then being $E_{n,\mathrm{p,o}}$, the name 'photon fluence rate, amount basis', SI unit is $\mathrm{mol\ m^{-2}\ s^{-1}}$; common unit is $\mathrm{einstein\ m^{-2}\ s^{-1}}$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 395

photon flux, q_p, Φ_p

Number of photons (quanta of radiation, N_p) per time interval. SI unit is s^{-1}.
Notes:

1. Mathematical definition: $q_p = dN_p / dt$. If the number of photons is constant over the time interval, $q_p = N_p / t$.
2. This quantity can be used on a chemical amount basis by dividing the photon flux, number basis, q_p, by the Avogadro constant, the symbol then being $q_{n,p}$, the name 'photon flux, amount basis', SI unit is mol s^{-1}; common unit is einstein s^{-1}.
3. Although the symbol recommended by CEI is Φ_p, the symbol q_p is preferred since Φ is reserved for quantum yield.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 395

photon irradiance, E_p

Number of photons (quanta of radiation, N_p) per time interval (photon flux), q_p, incident from all upward directions on a small element of surface containing the point under consideration divided by the area of the element. SI unit is $m^{-2}\ s^{-1}$. Equivalent definition: Integral, taken over the hemisphere visible from the given point, of the expression $L_p \cos\theta\ d\Omega$ the photon radiance at the given point in the various directions of the incident beam of solid angle Ω and θ the angle between any of these beams and the normal to the surface at the given point.
Notes:

1. Mathematical definition: $E_p = dq_p / dS$. If the photon flux is constant over the surface considered, $E_p = q_p / S$. Equivalent definition: $E_p = \int_{2\pi} L_p \cos\theta d\Omega$.
2. This term refers to a beam not scattered or reflected by the target or its surroundings. For a beam incident from all directions photon fluence rate ($E_{p,o}$) is an equivalent term.
3. This quantity can be used on a chemical amount basis by dividing E_p by the Avogadro constant, the symbol then being $E_{n,p}$, the name 'photon irradiance, amount basis', SI unit is $\text{mol m}^{-2}\ s^{-1}$; common unit is $\text{einstein m}^{-2}\ s^{-1}$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 396

photon number, N_p

Total number of photons calculated as $N_p = n_p N_A$ with N_p the amount of photons in einsteins and N_A the Avogadro constant.
Note:
Mathematical definition: $N_p = Q/_{h\nu}$ for monochromatic radiation of frequency ν, with Q the radiant energy.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 396

photon quantities

A group of quantities characterizing electromagnetic radiation in terms of the number of photons. The symbols of photon quantities may be distinguished by adding a subscript p.
See also: radiant, luminous quantities

Source:
Green Book, 2nd ed., p. 30

photon radiance, L_p

Number of photons (quanta of radiation, N_p) per time interval (photon flux), q_p, leaving or passing through a small transparent element of surface in a given direction from the source about the solid angle Ω, divided by the solid angle and by the orthogonally projected area of the element in a plane normal to the given beam direction, $\mathrm{d}S_\perp = \mathrm{d}S\cos\theta$, with θ the angle between the normal to the surface and the direction of the beam. Equivalent definition: Integral taken over the hemisphere visible from the given point, of the expression $L_p \cos\theta \, \mathrm{d}\Omega$, with L_p the photon radiance at the given point in the various directions of the incident beam of solid angle Ω and θ the angle between any of these beams and the normal to the surface at the given point.
Notes:

1. Mathematical definition:

$$L_p = \frac{\mathrm{d}^2 q_p}{\mathrm{d}\Omega\,\mathrm{d}S_\perp} = \frac{\mathrm{d}^2 q_p}{\mathrm{d}\Omega\,\mathrm{d}S\cos\theta}$$

   for a divergent beam propagating in an elementary cone of the solid angle Ω containing the direction θ. SI unit is $\mathrm{m}^{-2}\,\mathrm{s}^{-1}\,\mathrm{sr}^{-1}$.
2. For a parallel beam it is the number of photons (quanta of radiation, N_p) per time interval (photon flux), q_p, leaving or passing through a small element of surface in a given direction from the source divided by the orthogonally projected area of the element in a plane normal to the given direction of the beam, θ. Mathematical definition in this case: $L_p = \mathrm{d}q_p / (\mathrm{d}S\cos\theta)$ If q_p is constant over the surface area considered, $L_p = q_p / (S\cos\theta)$, SI unit is $\mathrm{m}^{-2}\,\mathrm{s}^{-1}$.

3. This quantity can be used on a chemical amount basis by dividing L_p by the Avogadro constant, the symbol then being $L_{n,p}$, the name 'photon radiance, amount basis'. For a divergent beam SI unit is $\text{mol m}^{-2}\text{ s}^{-1}\text{ sr}^{-1}$; common unit is $\text{einstein m}^{-2}\text{ s}^{-1}\text{ sr}^{-1}$. For a parallel beam SI unit is $\text{mol m}^{-2}\text{ s}^{-1}$; common unit is $\text{einstein m}^{-2}\text{ s}^{-1}$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 396

photooxidation

Oxidation reactions induced by light. Common processes are: 1, the loss of one or more electrons from a chemical species as a result of photoexcitation of that species; 2, the reaction of a substance with oxygen under the influence of light. When oxygen remains in the product this latter process is also called photooxygenation. Reactions in which neither the substrate nor the oxygen are electronically excited are sometimes called photoinitiated oxidations.
See also: photoreduction

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2264

photooxygenation

The incorporation of molecular oxygen into a molecular entity. There are three common mechanisms: Type I: the reaction of triplet molecular oxygen with radicals formed photochemically. Type II: the reaction of photochemically produced singlet molecular oxygen with molecular entities to give rise to oxygen containing molecular entities. The third mechanism proceeds by electron transfer producing superoxide anion as the reactive species.
See also: photooxidation

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2264

photophoresis

In aerosol physics, the motion of particles due to the influence of light. In many cases, this amounts to a special form of thermophoresis due to the heating of the particles by the light.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2206

photophosphorylation

The transformation of light (solar) energy for the reduction of CO_2 and the generation of adenosine 5'-triphosphate, ATP.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

photophysical processes

Photoexcitation and subsequent events which lead from one to another state of a molecular entity through radiation and radiationless transitions. No chemical change results.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2264

photopolymerization

Polymerization processes requiring a photon for the propagation step.
See also: photoinduced polymerization

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2264

photorearrangement

Photoisomerization involving changes in the arrangement of the atoms within the molecular species. It may lead to unstable isomers that react further by, e.g., dehydrogenation, deprotonation, or other reactions.
Note:
Examples are photorearrangements of alkenes (other than *cis*-*trans* photoisomerization), of cyclohex-2-enones, of endoperoxides, of thioarenes, the di-π-methane rearrangement and others.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 398

photoreduction

Reduction reactions induced by light. Common processes are: 1, addition of one or more electrons to a photoexcited species; 2, the photochemical hydrogenation of a substance. Reactions in which the substrate is not electronically excited are sometimes called photoinitiated reductions.
See also: photooxidation

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2264

photoresist

A photoimaging material, generally applied as a thin film, whose local solubility properties can be altered photochemically. A subsequent development step produces an image which is useful for the fabrication of microelectronic devices (e.g. integrated circuits).

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2265

photoselection

Selection of an aligned subset of sample molecules by an exciting light beam. The selected subset will have an orientation distribution that is determined by the electric vector of the beam. If the beam is linearly polarized a uniaxial sample with a known orientation distribution will be produced. Also, the set of remaining molecules will be aligned with a known orientation distribution (residual anisotropy).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 399

photosensitive polymer

Polymer that responds to ultraviolet or visible light by exhibiting a change in its physical properties or its chemical constitution.
Notes:
1. Examples of the changes in photosensitive polymers are a change in molecular shape (photo-responsive polymer), a change in its constitution (photo-reactive polymer), and a reversible change in color (photochromic polymer).
2. Photosensitivity in photosensitive polymers means that the polymers are sensitive to the irradiated light leading to some change in properties or structure. It is different from photosensitization.
3. ***See also:*** photoreaction, photochromism.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 901

photosensitization

The process by which a photochemical or photophysical alteration occurs in one molecular entity as a result of initial absorption of radiation by another molecular entity called a photosensitizer. In mechanistic photochemistry the term is limited to cases in which the photosensitizer is not consumed in the reaction.

See: energy transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2265
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 762

photosensitizer

See: photosensitization

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2265
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 762

photostationary state

A steady state reached by a reacting chemical system when light has been absorbed by at least one of the components. At this state the rates of formation and disappearance are equal for each of the transient molecular entities formed.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2265

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2206

photosynthesis

A metabolic process involving plants and some types of bacteria (e.g. Chromataceae, Rhodospirillaceae, Chlorobiaceae) in which light energy absorbed by chlorophyll and other photosynthetic pigments results in the reduction of CO_2 followed by the formation of organic compounds. In plants the overall process involves the conversion of CO_2 and H_2O to carbohydrates (and other plant material) and the release of O_2 .

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2207
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

photosystem

A membrane-bound complex in plants and photosynthetic bacteria, responsible for light-harvesting and primary electron transfer. Comprises light-harvesting pigments such as chlorophyll; a primary electron-transfer centre, and secondary electron carriers. In green plant photosynthesis, Photosystem I transfers electrons from plastocyanin to a [2Fe-2S] ferredoxin, and contains iron-sulfur proteins. Photosystem II transfers electrons from the oxygen-evolving complex to plastoquinone, and contains an iron centre.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1292

photothermal effect

An effect produced by photoexcitation resulting partially or totally in the production of heat.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2265

photothermography

A process utilizing both light and heat, simultaneously or sequentially, for image recording.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2265

phototransistor

Also contains definitions of: Darlington phototransistor, field effect phototransistor

A bipolar transistor with its base-collector junction acting as a photodiode, which, if irradiated, controls the response of the device. Due to the inherent current gain (of the transistor) the responsivity of the phototransistor is greater than that of photodiodes. A Darlington phototransistor consists of two separate transistors coupled in the high-impedance Darlington configuration with a phototransistor as the input transistor. A field effect phototransistor or photo-FET is a field effect transistor (FET) that employs photogeneration of carriers in the channel region (the neutral region sandwiched between the insulator and the depletion region under the gate of the FET). It is characterized by high responsivity due to the high current gain of the FET.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1755

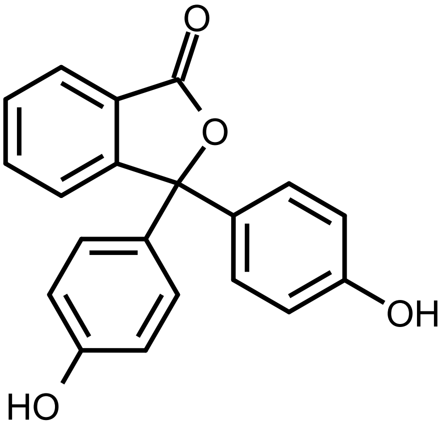
photovoltaic cell

A solid state device, usually a semiconductor such as silicon, which absorbs photons with energies higher than or equal to the bandgap energy and simultaneously produces electric power.
See also: photogalvanic cell

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2265
PAC, 1991, *63*, 569 *(Terminology in semiconductor electrochemistry and photoelectrochemical energy conversion (Recommendations 1991))* on page 593

phthaleins

3,3-Bis(hydroxyaryl)-2-benzofuran-1(3*H*)-ones generally derived from the condensation of phthalic anhydride with phenols. E.g. phenolphthalein.



phenolphtalein

See: xanthenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

phthalides

3,3-Di(hydrocarbyl) or 3-hydrocarbylidene-2-benzofuran-1(3*H*)-ones.
See: phthaleins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

physical network

Polymer network with junction points or zones formed by physically interacting chains which need not be permanent.
Notes:
1. The junction points or zones need not be permanent over the time scale of the observation or measurement.
2. The interaction can be due to hydrogen bonds, π–π interactions, chain entanglements, *etc.*

3. Modification of the entry given as a note within the definition of network in polymer chemistry.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1815

physical quantity (measurable quantity)

An attribute of a phenomenon, body or substance that may be distinguished qualitatively and determined quantitatively.

Source:
Green Book, 2nd ed., p. 3
VIM

physisorption (physical adsorption)

Adsorption in which the forces involved are intermolecular forces (van der Waals forces) of the same kind as those responsible for the imperfection of real gases and the condensation vapours, and which do not involve a significant change in the electronic orbital patterns of the species involved. The term van der Waals adsorption is synonymous with physical adsorption, but its use is not recommended.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 586
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 75

phytotoxicant

An agent which produces a toxic effect in vegetation.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2207

pico

SI prefix for 10^{-12} (symbol: p).

Source:
Green Book, 2nd ed., p. 74
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 987

picrates

Salts or charge-transfer complexes of picric acid (2,4,6-trinitrophenol).
See: styphnates

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

piezoelectric polymer

1. Polymer that exhibits a change in dielectric properties on application of pressure or
2. polymer that shows a change in its dimensions when subjected to an electric field.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 901

piezoluminescence

Luminescence observed when certain solids are subjected to a change in pressure.
See: triboluminescence

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2265

pile-up

in radioanalytical chemistry

The processing by a radiation spectrometer of pulses resulting from the simultaneous adsorption of independent particles or photons in a radiation detector. As a result they are counted as one single particle or photon with energy between the individual energies and the sum of these energies.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523
Orange Book, p. 235

PIN semiconductor detector

A semiconductor detector consisting of a compensated region between a p and a n region. The compensated region is often referred to as intrinsic.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552

pinacols

Tetra(hydrocarbyl)ethane-1,2-diols, $R_2C(OH)–(OH)R_2$, of which the tetramethyl example is the simplest one and is itself commonly known as pinacol (benzpinacol is the tetraphenyl analogue).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

pinocytosis

Type of endocytosis in which soluble materials are taken up by the cell and incorporated into vesicles for digestion.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1065

pitch

A residue from pyrolysis of organic material or tar distillation which is solid at room temperature, consisting of a complex mixture of numerous, essentially aromatic hydrocarbons and heterocyclic compounds. It exhibits a broad softening range instead of a defined melting temperature. When cooled from the melt, pitches solidify without crystallization.
Note:
The ratio of aromatic to aliphatic hydrogen depends mainly on the source of the starting material. The hydrogen aromaticity (ratio of aromatic to total hydrogen atoms) varies between 0.3 and 0.9. The aliphatic hydrogen in pitch is largely associated with alkyl side chains substituted on aromatic rings. The content of heterocyclic compounds in pitches varies depending on their origins. Also, the softening temperature can vary in a broad range between about 320 and $570\ \mathrm{K}$ depending on the molecular weight (relative molecular mass) and composition of the constituents.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 500

pitch-based carbon fibres

Carbon fibres obtained from pitch precursor fibres after stabilization treatment, carbonization and final heat treatment.
Note:
The term pitch-based carbon fibres comprises the isotropic pitch-based carbon fibres as well as the anisotropic mesophase pitch-based carbon fibres (MPP-based carbon fibres). The isotropic type belongs to the carbon fibres type LM (low modulus) and is mainly used as filler in polymers and insulation materials and for similar applications. The anisotropic type (MPP-based carbon fibres) belongs to the carbon fibres type HM and is used mainly for reinforcement purposes due to its high Young's modulus value.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 500

pitting corrosion

A special type of non-uniform corrosion of passive metals, resulting in the formation of pits, which usually occurs in the presence of certain anions at electrode potentials positive to a critical pitting potential.

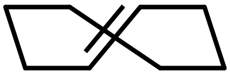
Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 22

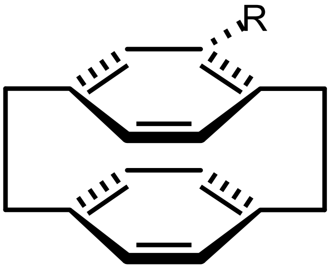
planar chirality

Also contains definition of: R_p, S_p

Synonym: planar stereoisomerism

Term used by some authorities to refer to stereoisomerism resulting from the arrangement of out-of-plane groups with respect to a plane (chirality plane). It is exemplified by the atropisomerism of (*E*)-cyclooctene (chiral plane = double bond and attached atoms) or monosubstituted paracyclophane (chiral plane = substituted ring). The configuration of molecular entities possessing planar chirality is specified by the stereodescriptors R_p and S_p (or P and M).





Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2213

planar chromatography

A separation technique in which the stationary phase is present as or on a plane. The plane can be a paper, serving as such or impregnated by a substrate as the stationary bed (paper chromatography, PC) or a layer of solid particles spread on a support e.g. a glass plate (thin layer chromatography, TLC). Sometimes planar chromatography is also termed open-bed chromatography.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 825

planar film

A film whose boundaries are represented by ideal parallel planes. The planar film thickness is defined as the distance between these planes. The terms nanometre thick film, micrometre thick film and millimetre thick film refer specifically to film thickness in the ranges $0.1 - 100\ \mathrm{nm}$, $0.1 - 100\ \mu\mathrm{m}$ and $0.1 - 100\ \mathrm{mm}$, respectively.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1671

planar intramolecular charge transfer

Acronym: PICT

In a PICT state formed by intramolecular charge transfer in an electron donor (D)/acceptor (A) molecule, the D and A subgroups have an overall planar configuration, with substantial electronic coupling of D and A.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 401

Planck constant

Universal fundamental physical constant $h = 6.626\ 06896(33) \times 10^{-34}\ \mathrm{J\ s}$, or $\hbar = \frac{h}{2\pi} = 1.054\ 571\ 628(53) \times 10^{-34}\ \mathrm{J\ s}$. The latter is used as atomic unit of action.

Source:
CODATA Bull. 1986, *63*, 1

plane angle

See: angle

Source:
Green Book, 2nd ed., p. 11
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 987

plasma desorption ionization

in mass spectrometry

The ionization of any species by interaction with heavy particles (which may be ions or neutral atoms) formed as a result of the fission of a suitable nuclide adjacent to a target supporting the sample.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548

plasma

in biology

1. Fluid component of blood in which the blood cells and platelets are suspended. Synonym: blood plasma
2. Fluid component of semen produced by the accessory glands, the seminal vesicles, the prostate, and the bulbo-urethral glands.
3. Cell substance outside the nucleus, *i.e.*, the cytoplasm.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1065

plasma

in spectrochemistry

A gas which is at least partly ionized and contains particles of various types, viz. electrons, atoms, ions and molecules. The plasma as a whole is electrically neutral.

Source:
Orange Book, p. 119

plasmid

An extrachromosomal genetic element consisting generally of a circular duplex of DNA which can replicate independently of chromosomal DNA. R-plasmids are responsible for the mutual transfer of antibiotic resistance among microbes. Plasmids are used as vectors for cloning DNA in bacteria or yeast host cells.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 162

plastic flow

Steady flow occurring only above a certain finite stress.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

plastic transition

A first-order transition that occurs when a low-temperature phase transforms to an orientationally-disordered high-temperature phase with a strong variation of enthalpy.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

plate height, H_{eff}

in chromatography

The column length (L) divided by the plate number:

$$H = \frac{L}{N}$$

It is also called the height equivalent to one theoretical plate (HETP).

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 848

plate number, N

Also contains definitions of: number of theoretical plates, theoretical plate number

in chromatography

A number indicative of column performance, calculated from the following equations which depend on the selection of the peak width expression:

$$N = \left(\frac{V_{\mathrm{R}}}{\sigma}\right)^2 = \left(\frac{t_{\mathrm{R}}}{\sigma}\right)^2$$

$$N = 16\left(\frac{V_{\mathrm{R}}}{w_{\mathrm{b}}}\right)^2 = 16\left(\frac{t_{\mathrm{R}}}{w_{\mathrm{b}}}\right)^2$$

$$N = 5.545\left(\frac{V_{\mathrm{R}}}{w_{\mathrm{h}}}\right)^2 = 5.545\left(\frac{t_{\mathrm{R}}}{w_{\mathrm{h}}}\right)^2$$

The value of 5.545 stands for $8\ \ln 2$. These expressions assume a Gaussian (symmetrical) peak. In these expressions the units for the quantities inside the brackets must be consistent so that their ratio is dimensionless: i.e. if the numerator is a volume, then peak width must also be expressed in terms of volume. In former nomenclature the expressions 'number of theoretical plates' or 'theoretical plate number' were used for the same term. For simplification, the present name is suggested.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 847

plateau border

in surface chemistry

Except for free-floating bubbles, films have to be supported by frames, bulk surfaces or other films. The transition zone separating these from the film proper, always containing some bulk liquid, is called a plateau border.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

PLED

Acronym for polymer light-emitting diode.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 401

pleiotropic gene

A gene affecting more than one (apparently unrelated) characteristic of the phenotype.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 163

ploidy

A term indicating the number of sets of chromosomes present in an organism, e.g. haploid (one) or diploid (two).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 163

plug-flow

in catalysis

A packed bed flow reactor is commonly called a fixed bed reactor and the term plug-flow is also used to indicate that no attempt is made to back-mix the reaction mixture as it passes through the catalyst bed.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

plumbylenes [obsolete]

An older, no longer recommended name for plumbylidenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

plumbylidenes

Carbene analogues having the structure $R_2Pb:$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

plume

in atmospheric chemistry

The gaseous and aerosol effluents which are emitted from a chimney and the volume of space which they occupy (often visible). The shape of the plume and the concentrations of pollutants in it at various points along the path of the plume are sensitive functions of the meteorology, local topography and the chemistry which occurs in the plume. Urban plumes are observed over many urban areas and downwind of these areas in which a combination of man sources of pollution are concentrated.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2207

plus, minus

See:
1. d, l, dl for (+), (−) and (±)
2. Helicity for *P* and *M*.

> ***Source:***
> PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2213

pneumatic detector

A pressure-sensitive detector based on the pressure increase of a gas. A special type is the Golay cell where the pressure change is detected by observing the deflection off one of the chamber walls.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1752

point group

The classification of the symmetry elements of an object. It is denoted in the Schoenflies notation by an italic symbol, such as C_3, D_2, T_d, etc.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2213

point of zero charge (p.z.c.)

A surface charge is at its point of zero charge when the surface charge density is zero. It is a value of the negative logarithm of the activity in the bulk of the charge-determining ions.

Source:
PAC, 1991, *63*, 895 *(Nomenclature, symbols, definitions and measurements for electrified interfaces in aqueous dispersions of solids (Recommendations 1991))* on page 902

poise

cgs unit of dynamic viscosity, $\mathrm{P} = 0.1\ \mathrm{Pa\ s}$.

Source:
Green Book, 2nd ed., p. 112
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 987

poison

in catalysis

An inhibitory substance characterized by its propensity to attach very strongly, by a true chemical bond (e.g. covalent) to the surface atoms or ions constituting the catalytically active sites. Poisons act in minute quantities. Typical poisons are S, As, etc. In most cases, activity and/or selectivity cannot be recovered without a drastic change in operating conditions (most often a regeneration). Recovery, if at all, takes place very slowly and/or only partially.

Source:
PAC, 1991, *63*, 1227 *(Manual on catalyst characterization (Recommendations 1991))* on page 1244

Poisson distribution

A discrete distribution with the differential mass-distribution function of the form:

$$f_{\mathrm{w}}(x) = \frac{x}{a+1} = \frac{\mathrm{e}^{-a}\, a^{x-1}}{(x-1)\,!}$$

where x is a parameter characterizing the chain length, such as relative molecular mass or degree of polymerization and a is a positive adjustable parameter.

Source:
Purple Book, p. 56

polar aprotic solvent [obsolete]

See: dipolar aprotic solvent

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1150

polar effect

For a reactant molecule RY, the polar effect of the group R comprises all the processes whereby a substituent may modify the electrostatic forces operating at the reaction centre Y, relative to the standard $R^{o}Y$. These forces may be governed by charge separations arising from differences in the electronegativity of atoms (leading to the presence of dipoles), the presence of unipoles, or electron delocalization. It is synonymous with electronic effect or 'electrical effect' of a substituent as distinguished from other substituent effects, e.g. steric effects. Sometimes, however, the term 'polar effect' is taken to refer to the influence, other than steric, that non-conjugated substituents exert on reaction rates, i.e. effects connected with electron delocalization between a substituent and the molecular framework to which it is attached are excluded. Polar effect is then not synonymous with electronic effect
See also: field effect, inductive effect, mesomeric effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1150

polar solvent

See: polarity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1151

polarity

When applied to solvents, this rather ill-defined term covers their overall solvation capability (solvation power) for solutes (i.e. in chemical equilibria: reactants and products; in reaction rates: reactants and activated complex; in light absorptions: ions or molecules in the ground and excited state), which in turn depends on the action of all possible, nonspecific and specific, intermolecular interactions between solute ions or molecules and solvent molecules, excluding such interactions leading to definite chemical alterations of the ions or molecules of the solute. Occasionally, the term solvent polarity is restricted to nonspecific solute/solvent interactions only (i.e. to van der Waals forces).

See also: Dimroth–Reichardt E_T parameter, Grunwald–Winstein equation, ionizing power, Kamlet–Taft solvent parameters, van der Waals forces, Z-value

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1151

polarizability

The ease of distortion of the electron cloud of a molecular entity by an electric field (such as that due to the proximity of a charged reagent). It is experimentally measured as the ratio of induced dipole moment (μ_{ind}) to the field E which induces it:

$$\alpha = \frac{\mu_{\text{ind}}}{E}$$

The units of α are $\mathrm{C^2\ m^2\ V^{-1}}$. In ordinary usage the term refers to the 'mean polarizability', i.e., the average over three rectilinear axes of the molecule. Polarizabilities in different directions (e.g. along the bond in Cl_2 , called 'longitudinal polarizability', and in the direction perpendicular to the bond, called 'transverse polarizability') can be distinguished, at least in principle. Polarizability along the bond joining a substituent to the rest of the molecule is seen in certain modern theoretical approaches as a factor influencing chemical reactivity, etc., and parametrization thereof has been proposed.
See also: electric polarizability

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1151

polarization, *P*

The relevant material property that couples with the radiation field. May be called optical or dielectric polarization. Optical spectroscopies may be classified according to the dielectric polarization power-law dependence on the external electric field.
Notes:

1. Mathematically it is defined as the electric dipole moment change per volume resulting from absorption of radiation of optical frequencies, defined as $\boldsymbol{P} = \boldsymbol{D} - \varepsilon_0 \boldsymbol{E}$, where $\boldsymbol{D}$ is the electric displacement, ε_0 the electric constant (vacuum permittivity) , and $\boldsymbol{E}$ the strength of the radiation electric field. A dielectric medium is characterized by the constitutive relation $\boldsymbol{D} = \varepsilon_0\, \chi^{(1)}$ where $\chi^{(1)} = \varepsilon_{\mathrm{r}} - 1$ is the linear 'susceptibility' for a transparent singly refracting medium. Depending on the molecular or atomic restoring force on the electron with respect to the displacement $\boldsymbol{D}$, the field-induced motion of the electron can introduce other frequency components on the electron motion, and this in turn leads to non-linear optical effects.
2. The polarization component to the *n*th-order in the field is denoted as $\boldsymbol{P}^{(\mathrm{n})}$ Thus, the following equations apply,
   $\boldsymbol{P} = \boldsymbol{P}^{(1)} + \boldsymbol{P}_{\mathrm{NL}}$ and $\boldsymbol{P}_{\mathrm{NL}} = \boldsymbol{P}^{(2)} + \boldsymbol{P}^{(3)} + \ldots$

$$\boldsymbol{P} = \varepsilon_0\,[\chi_{\mathrm{e}}^{(1)}\,\boldsymbol{E} + (1/2)\,\chi_{\mathrm{e}}^{(2)}\,\boldsymbol{E}^2 + (1/6)\,\chi_{\mathrm{e}}^{(3)}\,\boldsymbol{E}^3 + \ldots] = \boldsymbol{P}^{(1)} + \boldsymbol{P}^{(2)} + \boldsymbol{P}^{(3)} + \ldots$$

where $\boldsymbol{E}^i$ is the i-th component of the electric field strength and $\chi_{\mathrm{e}}^{(\mathrm{n})}$ is the usual 'susceptibility' $\chi^{(1)} = \varepsilon_{\mathrm{r}} - 1$ in the absence of higher terms and $\boldsymbol{P}^{(\mathrm{n})}$ is the order of the field-induced polarization in the material.

In an anisotropic medium, $\chi_{\mathrm{e}}^{(1)}$, $\chi_{\mathrm{e}}^{(2)}$ and $\chi_{\mathrm{e}}^{(3)}$ are the medium 'hyper-susceptibilities'; they are tensors of rank 2, 3, and 4, respectively.

Linear optical responses such as absorption, light propagation, reflection, and refraction, involving a weak incoming field, are related to $\boldsymbol{P}^{(1)}$. Non-linear techniques are connected to the non-linear polarization $\boldsymbol{P}_{\mathrm{NL}}$. Low order non-linear techniques, such as three-wave mixing, are related to the second order optical polarization $\boldsymbol{P}^{(2)}$. For a random isotropic medium (such as a liquid) or for a crystal with a centrosymmetric unit cell, $\chi_{\mathrm{e}}^{(2)}$ is zero by symmetry and then the lowest order non-linear techniques, as well as the higher order, are related to the third-order optical polarization, $\boldsymbol{P}^{(3)}$, and the corresponding hyper-susceptibility.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 402

polarization error

in spectrochemical analysis

An error which arises from the fact that the absorbance of a sample (especially a solid) could depend on the polarization of the incident radiation and from the polarization dependent response of the photodetector.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1456

polarization, ζ

in electrochemistry

The difference of the electrode potential from the corrosion potential. The symbol should not be used for polarization.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

polarized interphases

Ideally, interphases for which there are no common components between the phases or the exchange of these is hindered.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1253

polarography

A measure of current as a function of potential when the working electrode is a dropping mercury (or other liquid conductor) electrode and unstirred solutions are used.

Source:
Orange Book, p. 76

polaron

Lattice distortion or polarization caused by photoexcitation.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 403

pollution (pollutant)

See: air pollutant, air pollution

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2172

polyacid

In polymer terminology, polyelectrolyte composed of macromolecules containing acid groups on a substantial fraction of the constitutional units.
Note:
Most commonly, the acid groups are $–COOH$, $–SO_3H$, or $–PO_3H_2$.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2072

polyaddition

A polymerization in which the growth of polymer chains proceeds by addition reactions between molecules of all degrees of polymerization.
Notes:
1. The growth steps are expressed by:

$$\mathrm{P}_x + \mathrm{P}_y \rightarrow \mathrm{P}_{x+y} \qquad \{x\} \in \{1, 2, ...\infty\}; \{y\} \in \{1, 2, ...\infty\}$$

where P_x and P_y denote chains of degrees of polymerization x and y, respectively.

2. The earlier term 'addition polymerization' embraced both the current concepts of 'polyaddition' and 'chain polymerization', but did not include 'condensative chain polymerization'.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2307

polybase

In polymer terminology, polyelectrolyte composed of macromolecules containing basic groups on a substantial fraction of the constitutional units.
Note:
Most commonly, the basic groups are amino groups.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2072

polybetaine

Ampholytic polymer in which pendant groups have a betaine-type structure.
Note:
A polybetaine is a type of zwitterionic polymer.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2072

polychromator

An extension of a monochromator, a number of exit slits being placed in the focal plane, so allowing a number of discrete bands to pass through (to fall, for example, upon a number of photomultipliers).

Source:
Orange Book, p. 156

polycondensation

A polymerization in which the growth of polymer chains proceeds by condensation reactions between molecules of all degrees of polymerization.
Notes:

1. The growth steps are expressed by:

$$\mathrm{P}_x + \mathrm{P}_y \rightarrow \mathrm{P}_{x+y} + \mathrm{L} \qquad \{x\} \in \{1, 2, ...\infty\}; \{y\} \in \{1, 2, ...\infty\}$$

where P_x and P_y denote chains of degree of polymerization x and y, respectively, and L a low-molar-mass by-product.

2. The earlier term 'polycondensation' was synonymous with 'condensation polymerization'. It should be noted that the current definitions of polycondensation and condensative chain polymerization were both embraced by the earlier term 'polycondensation'.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2307

polycrystalline graphite

A graphite material with coherent crystallographic domains of limited size regardless of the perfection and preferred orientation (texture) of their crystalline structure.
Note:
The common use of the term polycrystalline graphite for polygranular graphite is in line with this definition but may be inexact because usually all grains of polygranular graphite are polycrystalline themselves. Polycrystalline graphite can exhibit a random orientation, more or less preferred orientation, or a highly oriented texture as in some pyrolytic graphites There is no sharp transition, however, between the typical polycrystalline texture and the 'single crystal-like' texture of highly oriented pyrolytic graphite (HOPG).

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 500

polycyclic system

A molecular system regarded as containing a number of rings equal to the number of scissions required to convert it into an open-chain compound.

Source:
Blue Book, p. 33

polydisperse medium

A colloidal system in which many particle sizes occur.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

polydisperse polymer

See: non-uniform polymer

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2302

polyelectrolyte

Synonyms: polymer electrolyte, polymeric electrolyte

Polymer composed of macromolecules in which a substantial portion of the constitutional units contains ionic or ionizable groups, or both.
Notes:
1. The terms polyelectrolyte, polymer electrolyte, and polymeric electrolyte should not be confused with the term solid polymer electrolyte.
2. Polyelectrolytes can be either synthetic or natural. Nucleic acids, proteins, teichoic acids, some polypeptides, and some polysaccharides are examples of natural polyelectrolytes.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2072

polyelectrolyte complex

Neutral polymer-polymer complex composed of macromolecules carrying charges of opposite sign causing the macromolecules to be bound together by electrostatic interactions.
Note:
A polyelectrolyte complex is also called a polysalt. Use of this term is not recommended.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2073

polyelectrolyte gel

Polymer gel in which the polymer network contains ionic or ionizable groups in a significant fraction of its constitutional units.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1808

polyelectrolyte network

Polymer network containing ionic or ionizable groups in a substantial fraction of its constitutional units.
Notes:
1. A polyelectrolyte network is sometimes called a crosslinked polyelectrolyte. Use of the latter term is not recommended unless the polyelectrolyte network is formed by the crosslinking of existing polyelectrolyte macromolecules rather than by non-linear polymerisation
2. In contrast to a polyelectrolyte, a polyelectrolyte network is always insoluble, although swelling or contraction can occur when it is immersed in a solvent.
3. A polyelectrolyte network in contact with a solution of a salt is able to exchange counter-ions (cations or anions) with ionic species in the solution and act as an ion exchanger. Therefore, a polyelectrolyte network is frequently described as an ion-exchange polymer.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2073

polyfunctional catalysis

See: bifunctional catalysis

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 78

polygranular carbon

A carbon material composed of grains, which can be clearly distinguished by means of optical microscopy.
Note:
Industrial carbon materials (such as electrodes) are mostly polygranular, but special grades are agranular materials, such as glass-like carbon, carbon fibres or pyrolytic carbon. Such materials are covered by the term agranular carbon.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 501

polygranular graphite

A graphite material composed of grains which can be clearly distinguished by means of optical microscopy.
Note:
From the viewpoint of crystallinity, a polygranular graphite is always a polycrystalline graphite but not vice versa. Most industrial graphite materials are polygranular. Monogranular materials consist mostly of non-graphitic carbon, such materials are called monolithic or agranular carbons.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 501

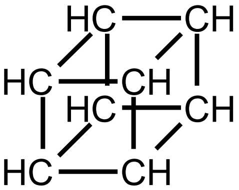
polyhedral symbol

The polyhedral symbol indicates the geometrical arrangements of the coordinating atoms about the central atom. It consists of one or more capital italic letters derived from common geometric terms (tetrahedron, square plane, octahedron, etc.) which denote the idealised geometry of the ligands around the coordination centre, and an arabic numeral that is the coordination number of the central atom. The polyhedral symbol is used as an affix, enclosed in parentheses, and separated from the name by a hyphen. Examples are *T*-4, *SP*-4, *TBPY*-5, *SPY*-5, *OC*-6, and *CU*-8.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1292

polyhedranes

Polycyclic hydrocarbons of the $(CH)_n$ series having skeletons corresponding to the regular and semiregular geometrical solids, e.g. cubane,



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

polyions

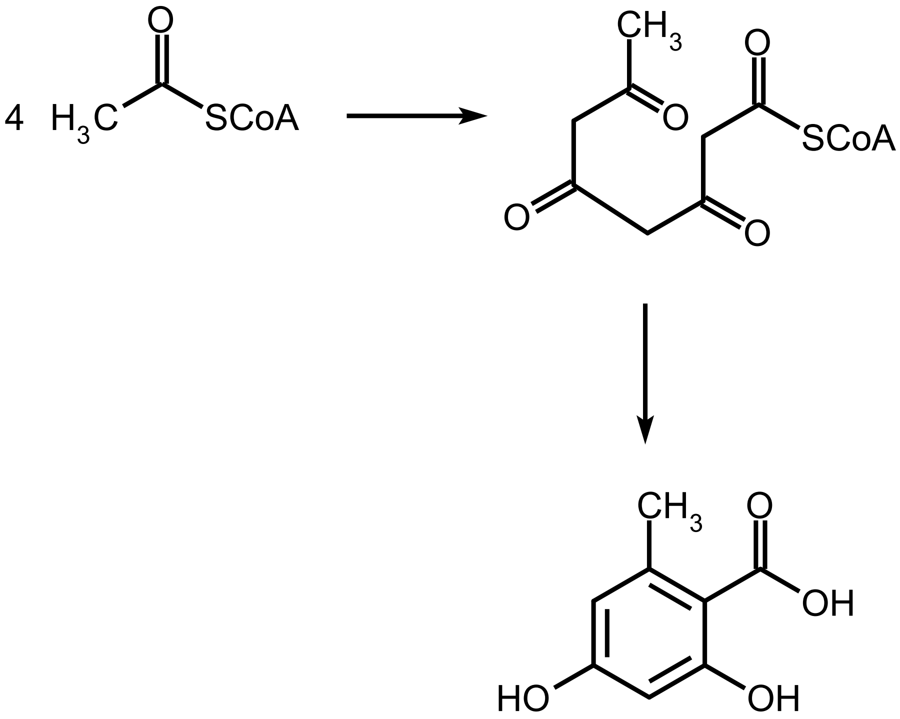
Polycations or polyanions — multiply charged ions.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 607

polyketides

Synonyms: acetogenins, ketides

Natural compounds containing alternating carbonyl and methylene groups ('β-polyketones'), biogenetically derived from repeated condensation of acetyl coenzyme A (via malonyl coenzyme A), and usually the compounds derived from them by further condensations. Considered by many to be synonymous with the less frequently used terms acetogenins and ketides.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359

polymer

A substance composed of macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2289

polymer alloy

Polymeric material, exhibiting macroscopically uniform physical properties throughout its whole volume, that comprises a compatible polymer blend, a miscible polymer blend or a multiphase copolymer.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1816

polymer blend

Macroscopically homogeneous mixture of two or more different species of polymer.
Notes:

1. In most cases, blends are homogeneous on scales larger than several times the wavelengths of visible light.
2. In principle, the constituents of a blend are separable by physical means.
3. No account is taken of the miscibility or immiscibility of the constituent macromolecules, *i.e.*, no assumption is made regarding the number of phase domains present.
4. The use of the term polymer alloy for a polymer blend is discouraged, as the former term includes multiphase copolymers but excludes incompatible polymer blends.
5. The number of polymeric components which comprise a blend is often designated by an adjective, *viz.* binary, ternary, quaternary, *etc.*

Source:
PAC, 2007, *79*, 1801 ***(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))*** on page 1817

polymer catalyst

Polymer that exhibits catalytic activity.
Notes:
1. Certain synthetic polymer catalysts can behave like enzymes.
2. Poly(4-vinylpyridine) in its basic form, and sulfonated polystyrene in its acid form, are examples of polymers that can act as catalysts in some base- and acid-catalyzed reactions, respectively.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 896

polymer compatibilizer

Polymeric additive that, when added to a blend of immiscible polymers, modifies their interfaces and stabilizes the blend.
Note:
Typical polymer compatibilizers are block or graft copolymers.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 901

polymer complexation

Also contains definition of: polymer complex formation

Process that results in the formation of a polymer–polymer complex or a complex composed of a polymer and a low-molar-mass substance.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 893

polymer composite

Composite in which at least one component is a polymer.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1990

polymer crystal

A crystalline domain usually limited by well-defined boundaries.
Notes:

1. Polymer crystals frequently do not display the perfection that is usual for low-molar-mass substances.
2. Twinned polymer crystals are, sometimes, erroneously referred to as 'crystals'.
3. Polymer crystals that can be manipulated individually are often called (polymer) single crystals. A single crystal may contain different fold domains.

Source:
Purple Book, p. 76

polymer crystallite

A small crystalline domain. A crystallite may have irregular boundaries and parts of its constituent macromolecules may extend beyond its boundaries. This definition is not identical with that used in classical crystallography.

Source:
Purple Book, p. 76

polymer cyclization

Chemical reaction that leads to the formation of ring structures in or from polymer chains.
Notes:

1. Examples of cyclization along polymer chains are: (a) cyclization of polyacrylonitrile, (b) acetalization of poly(vinyl alcohol) with an aldehyde, (c) cyclization of polymers of conjugated dienes, such as polyisoprene or polybutadiene, leading to macrocycles.
2. Examples of cyclization of polymer molecules are: (a) cyclization of poly(dimethylsiloxane), (b) back-biting reaction during ionic polymerizations of heterocyclic monomers.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 893

polymer degradation

Chemical changes in a polymeric material that usually result in undesirable changes in the in-use properties of the material.

Notes:

1. In most cases (*e.g.*, in vinyl polymers, polyamides) degradation is accompanied by a decrease in molar mass. In some cases (*e.g.*, in polymers with aromatic rings in the main chain), degradation means changes in chemical structure. It can also be accompanied by crosslinking.
2. Usually, degradation results in the loss of, or deterioration in, useful properties of the material. However, in the case of biodegradation (degradation by biological activity), polymers may change into environmentally acceptable substances with desirable properties.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 893

polymer drug

Polymer that contains either chemically-bound drug molecules or pharmacologically active moieties.
Note:
A polymer drug is usually used to provide drug-delivery targeted to an organ and controlled release of an active drug at the target organ.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 902

polymer functionalization

Introduction of desired chemical groups into polymer molecules to create specific chemical, physical, biological, pharmacological, or other properties.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 894

polymer gel

Gel in which the network component is a polymer.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1808

polymer membrane

Thin layer of polymeric material that acts as a barrier permitting mass transport of selected species.
Note:
See also: membrane

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 902

polymer network

See: network polymer

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2305

polymer phase-transfer catalyst

Polymer that acts as a phase-transfer catalyst and thereby causes a significant enhancement of the rate of a reaction between two reactants located in neighboring phases owing to its catalysis of the extraction of one of the reactants across the interface to the other phase where the reaction takes place.
Notes:

1. Polymer phase-transfer catalysts in the form of beads are often referred to as triphase catalysts because such catalysts form the third phase of the reaction system.
2. ***See also:*** phase-transfer catalyst.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 896

polymer reactant

Also contains definitions of: polymer reagent, polymer-supported reagent

Reactant (reagent) that is or is attached to a high-molar-mass linear polymer or a polymer network.
Note:
The attachment may be by chemical bonds, by weaker interactions such as hydrogen bonds, or simply by inclusion.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 897

polymer reaction

Chemical reaction in which at least one of the reactants is a high-molar-mass substance.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 894

polymer solvent

Polymer that acts like a solvent for compounds of low molar mass.
Note:
An example of a polymer solvent is poly(oxyethylene); it can dissolve various inorganic salts by complexation.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 902

polymer sorbent

Polymer that adsorbs or absorbs a certain substance or certain substances from a liquid or a gas.
Notes:

1. A polymer sorbent may be a polymer adsorbent or a polymer absorbent. The former acts by surface sorption and the latter by bulk sorption.
2. ***See also:*** sorption, adsorption, absorption.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 902

polymer support

Polymer to or in which a reagent or catalyst is chemically bound, immobilized, dispersed, or associated.
Notes:

1. A polymer support is usually a network polymer.
2. A polymer support is usually prepared in bead form by suspension polymerization.
3. The location of active sites introduced into a polymer support depends on the type of polymer support. In a swollen-gel-bead polymer support the active sites are distributed uniformly throughout the beads, whereas in a macroporous-bead polymer support they are predominantly on the internal surfaces of the macropores.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 902

polymer surfactant

Polymer that lowers the surface tension of the medium in which it is dissolved, or the interfacial tension with another phase, or both.
Note:
See also: surfactant.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 903

polymer-derived ceramic

Acronym: PDC

Ceramic derived from a polymeric ceramic precursor.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1817

polymer-metal complex

Complex comprising a metal and one or more polymeric ligands.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 896

polymer-poor phase

Synonym: dilute phase *in polymer chemistry*

That phase of a two-phase equilibrium system, consisting of a polymer and low molecular weight material, in which the polymer concentration is lower. The use of the name 'sol phase' is discouraged. Synonymous with dilute phase.

Source:
Purple Book, p. 68

polymer-rich phase

Synonym: concentrated phase *in polymer chemistry*

That phase of a two-phase equilibrium system, consisting of a polymer and low molecular weight material, in which the polymer concentration is higher. The use of the name 'gel phase' is discouraged. Synonymous with concentrated phase.

Source:
Purple Book, p. 68

polymer-supported catalyst

Catalyst system comprising a polymer support in which catalytically active species are immobilized through chemical bonds or weaker interactions such as hydrogen bonds or donor–acceptor interactions.
Notes:

1. Polymer-supported catalysts are often based on network polymers in the form of beads. They are easy to separate from reaction media and can be used repeatedly.

2. Examples of polymer-supported catalysts are: (a) a polymer-metal complex that can coordinate reactants, (b) colloidal palladium dispersed in a swollen network polymer that can act as a hydrogenation catalyst.
3. Polymer-supported enzymes are a type of polymer-supported catalysts.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 896

polymer-supported reaction

Chemical reaction in which at least one reactant or a catalyst is bound through chemical bonds or weaker interactions, such as hydrogen bonds or donor–acceptor interactions, to a polymer.
Notes:
1. The easy separation of low-molar-mass reactants or products from the polymer-supported species is a great advantage of polymer-supported reactions.
2. Typical examples of polymer-supported reactions are: (a) reactions performed by use of polymer-supported catalysts, (b) solid-phase peptide synthesis, in which intermediate peptide molecules are chemically bonded to beads of a suitable polymer support.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 894

polymerase chain reaction (*PCR*)

A laboratory technique to rapidly amplify pre-determined regions of double-stranded DNA. Generally involves the use of a heat-stable DNA polymerase.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1293

polymeric sol

Sol in which the dispersed phase consists of particles having a polymeric structure.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1806

polymeric stationary phase (material)

in liquid chromatography

Stationary phase (material) based on particles of a cross-linked organic polymeric material. Typical materials are polystyrene divinylbenzene copolymers (PS-DVB) and modified *PS-DVB* materials.

Source:
PAC, 1997, *69*, 1475 *(Classification and characterization of stationary phases for liquid chromatography: Part I. Descriptive terminology (IUPAC Recommendations 1997))* on page 1479

polymerization

The process of converting a monomer mixture of monomers into a polymer

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2305

polymer–polymer complex

Complex, at least two components of which are different polymers.
Notes:

1. A complex is a molecular entity formed from two or more components that can be ionic or uncharged.
2. Although the intrinsic binding energy between the individual interacting sites giving rise to the complex is weaker than a covalent bond, the total binding energy for any single molecule may exceed the energy of a single covalent bond.
3. The properties of a complex defined here differ from those given elsewhere because, owing to the repeating nature of a polymer molecule, many interacting sites may be present, which together will provide stronger bonding than a single covalent bond.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1988

polymer–solvent interaction

The sum of the effects of all intermolecular interactions between polymer and solvent molecules in solution that are reflected in the Gibbs and Helmholtz energies of mixing.

Source:
Purple Book, p. 57

polymolecularity correction

A correction applied to relationships between a property and the molar mass or relative molecular mass, obtained from polymers non-uniform with respect to relative molecular mass, in order to obtain the corresponding relationship for polymers strictly uniform with respect to relative molecular mass.

Source:
Purple Book, p. 57

polymorphic transition

A reversible transition of a solid crystalline phase at a certain temperature and pressure (the inversion point) to another phase of the same chemical composition with a different crystal structure.
Note:
In a liquid-crystal transition, this term refers to phase changes in the smectic state or columnar discotic state.
Examples:

1. The transitions of SiO_2 (quartz-type) at $1143\ K$ to SiO_2 (tridymite-type), and at $1743\ K$ to SiO_2 (cristobalite-type).
2. The transition of β-AgI (wurtzite-type structure) to α-AgI (body-centred-cubic structure) at $418\ K$. Synonymous with enantiotropic transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 588

polypeptides

Peptides containing ten or more amino acid residues.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1359
White Book, p. 48

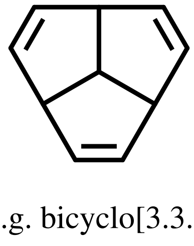
polyprenols

A subgroup of prenols in which n in the general formula $H–[CH_2–C(CH_3)=CH–CH_2]_n–OH$ is greater than 4.

Source:
PAC, 1987, *59*, 683 *(Nomenclature of prenols (Recommendations 1986))* on page 685
White Book, p. 252

polyquinanes (polyquinenes)

Saturated or unsaturated, respectively, polycyclic hydrocarbons consisting of fused five-membered rings, commonly but not necessarily incorporating the skeleton of quinacene (tricyclo[5.2.1.$0^{4,10}$]deca-2,5,8-triene):



E.g. bicyclo[3.3.0]octane, dodecahedrane.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1360

polysaccharides

Compounds consisting of a large number of monosaccharides linked glycosidically. This term is commonly used only for those containing more than ten monosaccharide residues. Also called glycans.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1360

polysulfanes

Compounds having an unbranched chain of sulfur atoms (S_2 or higher) terminating in H: HS_nH. Some chemists exclude disulfane, HS_2H, from the class polysulfanes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1360

polysulfides

Compounds $R{-}[S]_n{-}R$, with a chain of sulfur atoms ($n \geq 2$) and $R \neq H$. Some chemists exclude disulfides, RS_2R , from the class polysulfides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1360

polytopal rearrangement

Stereoisomerization interconverting different or equivalent spatial arrangements of ligands about a central atom or of a cage of atoms, where the ligand or cage defines the vertices of a polyhedron. For example pyramidal inversion of amines, Berry pseudorotation of PF_5, rearrangements of polyhedral boranes.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2213

polytypic transition

A transition of a crystalline structure into one or more forms which differ in the way identical layers of atoms are stacked. Example: ZnS consists of two identical close packings, one of Zn atoms, the other

S atoms, with the one displaced to the other along the *c*-axis through one-quarter of the layer spacing. In sphalerite-type ZnS the layers have the face-centred-cubic (ABC ABC) sequence, in wurtzite-type ZnS they have the hexagonal-close-packed (AB AB) sequence. The transition of sphalerite-type ZnS to wurtzite-type ZnS occurs at $1297\ \mathrm{K}$.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 589

pooled relative standard deviation

See: pooled standard deviation, relative standard deviation

Source:
PAC, 1981, *53*, 1805 *(Assignment and presentation of uncertainties of the numerical results of thermodynamic measurements (Provisional))* on page 1821

pooled standard deviation

A problem often arises when the combination of several series of measurements performed under similar conditions is desired to achieve an improved estimate of the imprecision of the process. If it can be assumed that all the series are of the same precision although their means may differ, the pooled standard deviations s_{p} from k series of measurements can be calculated as

$$s_{\mathrm{p}} = \sqrt{\frac{(n_1 - 1)\, s_1^{\,2} + (n_2 - 1)\, s_2^{\,2} + \ldots + (n_k - 1)\, s_k^{\,2}}{n_1 + n_2 + \ldots + n_k - k}}$$

The suffices $1,\ 2,\ \ldots,\ k$ refer to the different series of measurements. In this case it is assumed that there exists a single underlying standard deviation σ of which the pooled standard deviation s_{p} is a better estimate than the individual calculated standard deviations s_1, s_2, ..., s_k, For the special case where k sets of duplicate measurements are available, the above equation reduces to

$$s_{\mathrm{p}} = \sqrt{\frac{\sum (x_{i1} - x_{i2})^2}{2\,k}}$$

Results from various series of measurements can be combined in the following way to give a pooled relative standard deviation $s_{\mathrm{r,p}}$:

$$s_{\mathrm{r,p}} = \sqrt{\frac{\sum (n_i - 1)\, s_{\mathrm{r},i}^{\,2}}{\sum n_i - 1}} = \sqrt{\frac{\sum (n_i - 1)\, s_i^2\, x_i^{-2}}{\sum n_i - 1}}$$

Source:
PAC, 1981, *53*, 1805 *(Assignment and presentation of uncertainties of the numerical results of thermodynamic measurements (Provisional))* on page 1821

population inversion

A situation in which a higher energy state is more populated than a lower energy state.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

pore size distribution

The distribution of pore volume with respect to pore size; alternatively, it may be defined by the related distribution of pore area with respect to pore size.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

porosity

A concept related to texture, referring to the pore space in a material.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

porous-layer open-tabular (PLOT) column

in chromatography

A column in which there is a porous layer on the inner wall. Porosity can be achieved by either chemical means (e.g. etching) or by the deposition of porous particles on the wall from a suspension. The porous layer may serve as a support for a liquid stationary phase or as the stationary phase itself.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831

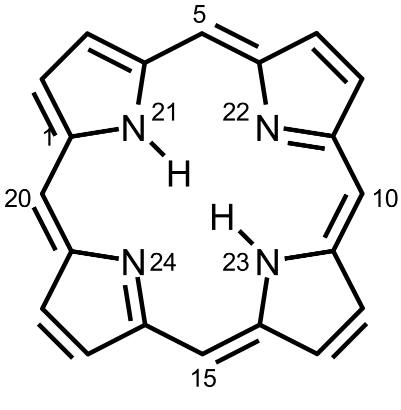
porphyrinogens

Hexahydroporphyrins in which the nitrogen atoms and four *meso* positions are saturated.

Source:
PAC, 1987, *59*, 779 *(Nomenclature of tetrapyrroles (Recommendations 1986))* on page 798
White Book, p. 294

porphyrins

Natural pigments containing a fundamental skeleton of four pyrrole nuclei united through the α-positions by four methine groups to form a macrocyclic structure (porphyrin is designated porphine in Chemical Abstracts indexes).



porphyrin

See also: corrinoids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1360
White Book, p. 281

position-sensitive photomultiplier tube

In position-sensitive photomultiplier tubes spatial resolution is obtained with the help of a partitioned photocathode.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1756

positive feedback

See: composite reaction

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 161

positive ion

in mass spectrometry

This is an atom, radical, molecule or molecular moiety which has lost one of more electrons thereby attaining an electrically positive charge. The use of the term cation as an alternative is not recommended. The use of mass ion is not recommended.
See: negative ion

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549

positron

A positively charged electron.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

positronium

Atom-like pair of particles consisting of an anti-electron (positron) and an electron.

Source:
Green Book, 2nd ed., p. 93

post-column derivatization

in chromatography

A version of reaction chromatography in which the separated components eluting from the column are derivatized prior to entering the detector. The derivatization process is generally carried out 'on-the-fly', i.e. during transfer of the sample components from the column to the detector. Derivatization may also be carried out before the sample enters the column or the planar medium; this is pre-column (preliminary) derivatization.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 827

post-filter effect

in luminescence spectroscopy

This effect arises when the exciting beam does not fill the cell completely and luminescence is absorbed by the analyte and interfering impurities in the non-illuminated region facing the detector.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 244

postprecipitation

The subsequent precipitation of a chemically different species upon the surface of an initial precipitate usually, but not necessarily, including a common ion.

Source:
Orange Book, p. 86

potential at the point of zero charge (p.z.c.)

The value of the electric potential of an electrode at which one of the charges defined is zero. The reference electrode against which this is measured should always be clearly stated. The potential difference with respect to the potential of zero charge is defined by

$$E_{\text{pzc}} = E - E_{\sigma=0}$$

where the potential at the point of zero charge is that for the given electrode in the absence of specific adsorption (other than that of the solvent).

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 509

potential energy, E_{p}, V

Energy of position or orientation in a field of force.

Source:
Green Book, 2nd ed., p. 12

potential of a cell reaction

See: standard electrode potential

Source:
Green Book, 2nd ed., p. 59

potential temperature

The temperature that a dry air parcel would have if lowered or raised adiabatically to a level of 1000 mbar pressure (or other arbitrary standard pressure).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2207

potential-determining (p.d.) ions

Those species which by virtue of their electron distribution between the solid and liquid phase (or by their equilibrium with electrons in the solid) determine the difference in Galvani potential between these phases. This definition requires that adsorbed p.d. ions are part of the adsorbent and belong to the category of surface ions.

Source:
PAC, 1991, *63*, 895 *(Nomenclature, symbols, definitions and measurements for electrified interfaces in aqueous dispersions of solids (Recommendations 1991))* on page 897

potential-energy profile

A curve describing the variation of the potential energy of the system of atoms that make up the reactants and products of a reaction as a function of one geometric coordinate, and corresponding to the 'energetically easiest passage' from reactants to products (i.e. along the line produced by joining the paths of steepest descent from the transition state to the reactants and to the products). For an elementary reaction the relevant geometric coordinate is the reaction coordinate ; for a stepwise reaction it is the succession of reaction coordinates for the successive individual reaction steps. (The reaction coordinate is sometimes approximated by a quasi-chemical index of reaction progress, such as 'degree of atom transfer' or bond order of some specified bond.)
See also: potential-energy (reaction) surface, Gibbs energy diagram

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1151
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 176

potential-energy (reaction) surface

A geometric hypersurface on which the potential energy of a set of reactants is plotted as a function of the coordinates representing the molecular geometries of the system. For simple systems two such coordinates (characterizing two variables that change during the progress from reactants to products) can be selected, and the potential energy plotted as a contour map. For simple elementary reactions, e.g. $\mathrm{A{-}B + C \rightarrow A + B{-}C}$, the surface can show the potential energy for all values of the A, B, C geometry, providing that the ABC angle is fixed. For more complicated reactions a different choice of two coordinates is sometimes preferred, e.g. the bond orders of two different bonds. Such a diagram is often arranged so that reactants are located at the bottom left corner and products at the top right. If the trace of the representative point characterizing the route from reactants to products follows two adjacent edges of the diagram, the changes represented by the two coordinates take place in distinct succession; if the trace leaves the edges and crosses the interior of the diagram, the two changes are concerted. In many qualitative applications it is convenient (although not strictly equivalent) for the third coordinate to represent the standard Gibbs energy rather than potential energy. Using bond orders is, however, an oversimplification, since these are not well-defined, even for the transition state. (Some reservations concerning the diagrammatic use of Gibbs energies are noted under Gibbs energy diagram). The energetically easiest route from reactants to products on the potential-energy contour map defines the potential-energy profile.

See also: reaction coordinate

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1151
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 177

potentiation

Dependent action in which a substance or physical agent at a concentration or dose that does not itself have an adverse effect enhances the harm done by another substance or physical agent.
See also: antagonism, synergism

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2085

potentiometer

1. In electronics, a sensitive voltage measuring device based on a null technique which provides infinite impedance at null.
2. In chemistry, potentiometric methods involve the measurement with a potentiometer of voltage generated in a cell. A high impedance digital voltmeter is often used today as a convenient alternative to a potentiometer.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2207

potentiometric detection method

in electrochemical analysis

A detection method in which the potential of a cell is related to the concentration (activity) of a reactant which is a component of the cell fluid.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2186

potentiometric selectivity coefficient

A coefficient which defines the ability of an ion-selective electrode to distinguish a particular ion from others. The selectivity coefficient, $K^{\mathrm{pot}}_{\mathrm{A,B}}$, is evaluated by means of the emf response of the ion-selective electrode in mixed solutions of the primary ion, A, and interfering ion, B (fixed interference method) or less desirable, in separate solutions of A and B (separate solution method). The activities of the primary ion, A, and the interfering ion, B, at which $K^{\mathrm{pot}}_{\mathrm{A,B}}$ is determined should always be specified, as the value of $K^{\mathrm{pot}}_{\mathrm{A,B}}$ is defined by the modified Nikolsky–Eisenman equation. The smaller the value of $K^{\mathrm{pot}}_{\mathrm{A,B}}$ the greater the electrode's preference for the principal ion, A. Comment: The terms selectivity constant and selectivity factor are frequently used instead of selectivity coefficient. However, in order to standardize the terminology associated with ion-selective electrodes, use of the term selectivity coefficient is recommended, as is the fixed interference method for its evaluation.This selectivity coefficient is not identical to the similar term used in separation science.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2532

power, *P*

Rate of energy transfer.

Source:
Green Book, 2nd ed., p. 13
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 987

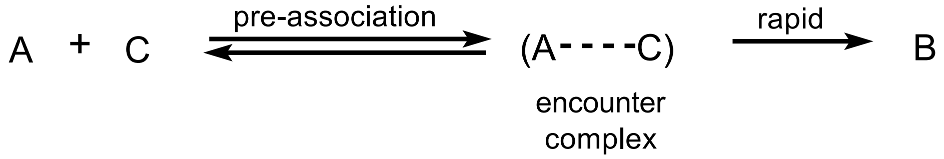
power level

Logarithm of the ratio of a power to a reference power. Levels are expressed in different ways: $L_P = \frac{1}{2}\ln\left(\frac{P}{P_0}\right)\ \mathrm{Np}$, where Np is the symbol for the unit neper coherent with the SI, or $L_P = 10\log_{10}\left(\frac{P}{P_0}\right)\ \mathrm{dB}$, where dB is the symbol for the unit decibel .

Source:
Green Book, 2nd ed., p. 79

pre-association

A step on the reaction path of some stepwise reactions in which the molecular entity C is already present in an encounter pair or encounter complex with A during the formation of B from A, e.g.



In this mechanism the chemical species C may but does not necessarily assist the formation of B from A, which may itself be a bimolecular reaction with some other reagent. Pre-association is important when B is too short-lived to permit B and C to come together by diffusion.
See also: microscopic diffusion control, spectator mechanism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1152

pre-equilibrium

in solvent extraction

1. Preliminary treatment of a solvent in order to convert the extractants into a suitable chemical form.
2. Preliminary treatment of either phase with a suitable solution of the other phase (in the absence of main extractable solute(s)) so that when the subsequent equilibration is carried out changes in the (volume) phase ratio or in the concentrations of other components are minimized.

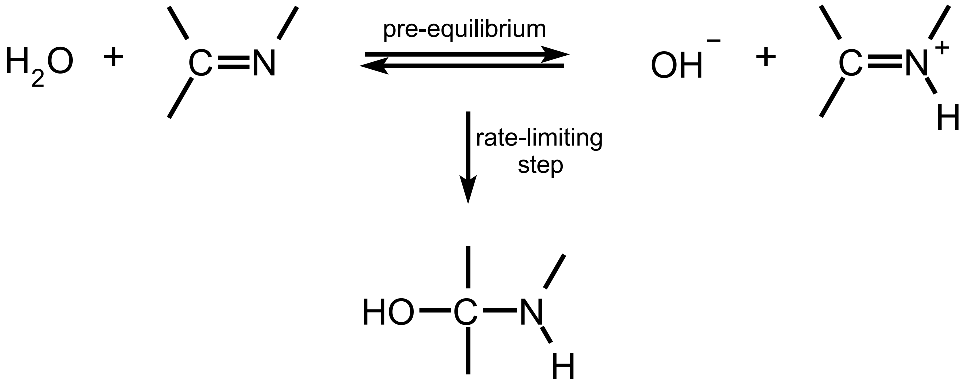
Notes:

1. The use of equilibration in this sense is confusing and should be avoided.
2. The term conditioning may be used as a synonym for pre-equilibration.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2378

pre-equilibrium (prior equilibrium)

A rapidly reversible step preceding the rate-limiting step in a stepwise reaction. For example:



See also: kinetic equivalence

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1152

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 177

pre-exponential factor, A

Also contains definition of: A-factor

Synonym: Arrhenius A factor

Coefficient in front of the exponential factor expressing the empirical temperature dependence of the rate coefficient, k, on temperature, T, $k = A\ \exp(-E_a / R\ T)$, where E_a is the activation energy.

Source:
Green Book, 2nd ed., p. 56
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 177

pre-filter effect

in luminescence spectroscopy

This effect arises when the luminescence detector does not see a portion of the luminescent volume where the excitation beam enters the sample. Thus the exciting beam flux is reduced by absorption by the analyte and interfering impurities before it enters the volume observed by the detection system.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 244

pre-gel regime

Stage of a network-forming polymerization or crosslinking process extending up to, but not beyond, the gel point.
Note:
The pre-gel regime may be expressed as the length of time or the chemical conversion required to reach the gel point from the start of a polymerization or crosslinking process.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1805

pre-gel state

State of a network-forming polymerization or crosslinking process in the pre-gel regime.
Note:
In the pre-gel state, the sol fraction is equal to unity. All the molecules formed have finite (statistically definable) relative molecular masses.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1805

pre-polymer

A polymer or oligomer composed of pre-polymer molecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2304

pre-polymer molecule

Also contains definition of: telechelic molecule

A macromolecule or oligomer molecule capable of entering, through reactive groups, into further polymerization, thereby contributing more than one monomeric unit to at least one chain of the final macromolecule. A pre-polymer molecule capable of entering into further polymerization through reactive end-groups, often deliberately introduced, is known as a telechelic molecule.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2290

pre-reactive complexes

Weakly bound complexes with a potential minimum that precedes the activation barrier along the reaction path. In contrast with the van der Waals complexes, which fall apart reversibly into their constituents, the pre-reactive complexes may undergo a vigorous reaction to form different products.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1958

precipitation

1. The sedimentation of a solid material (a precipitate) from a liquid solution in which the material is present in amounts greater than its solubility in the liquid.

   Source:
   PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2207

   See also:
   Orange Book, p. 84
   PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 589
2. Electrostatic precipitation: Separation of particles or droplets suspended in a gas or air. A large potential difference (12 to $30\,\mathrm{kV}$ dc) is required between the spaced electrodes in the precipitator. The charged particles are attracted to an electrode of opposite charge and collected.

   Source:
   PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2207

3. Precipitation (in meteorology): Rain, snowfall, hail, etc.

   Source:
   PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2207

precipitation fractionation

of polymers

A process in which a polymeric material, consisting of macromolecules differing in some characteristic affecting their solubility, is separated from solution into fractions by successively decreasing the solution power of the solvent, resulting in the repeated formation of a two-phase system in which the less soluble components concentrate in the polymer-rich phase.

Source:
Purple Book, p. 68

precipitation from homogeneous solution (pfhs)

in analysis

The formation of a precipitate which is generated homogeneously and, generally, slowly by a precipitating agent within a solution.

Source:
Orange Book, p. 84

precipitation

in sol-gel processing

Sedimentation of a solid material (a precipitate) from a liquid solution in which the material is present in amounts greater than its solubility in the liquid.
Note:
When precipitation occurs in sol-gel processing, sol particles have aggregated to a size where gravitational forces cause them to sink or float. Generally, aggregation arises from a change in the sol that reduces the interparticle repulsion.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1824

precision

The closeness of agreement between independent test results obtained by applying the experimental procedure under stipulated conditions. The smaller the random part of the experimental errors which affect the results, the more precise the procedure. A measure of precision (or imprecision) is the standard deviation.
Comment:

As recognized in VIM, precision is sometimes misused for accuracy. This problem will be avoided if one recognizes that precision relates only to dispersion, not to deviation from the (conventional) true value. Imprecision has been defined as 'the standard error of the reported value.'

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 598
VIM
Orange Book, p. 6
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2207

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

precision

of a balance

The standard deviation of the instrument for the stated load (e.g. l_{20} for a $20\ \mathrm{g}$ load). A statement of the procedure, conditions, and experience of the observer should be included.

Source:
Orange Book, p. 36

precision

of a weighing

This depends upon the method of weighing and upon the precision of indication, l, for the load in question.

Source:
Orange Book, p. 37

precision of indication

of a balance

The standard deviation of the instrumental indication, i, for a stated load.

Source:
Orange Book, p. 35

preconcentration coefficient

of a desired microcomponent

in trace analysis

This is defined as

$$K = \frac{Q_{\mathrm{T}}/Q_{\mathrm{M}}}{Q_{\mathrm{T}}^{\mathrm{o}}/Q_{\mathrm{M}}^{\mathrm{o}}}$$

where Q_{T} and $Q_{\mathrm{T}}^{\mathrm{o}}$ are the quantities of the microcomponent in the concentrate and in the sample, respectively (mass units or concentration units), and $Q_{\mathrm{M}}^{\mathrm{o}}$ and Q_{M} and are the quantities of the matrix before and after preconcentration, respectively. If the recovery is 100%, $K = \frac{Q_{\mathrm{M}}^{\mathrm{o}}}{Q_{\mathrm{M}}}$. The terms enrichment coefficient and enrichment factor are not recommended.

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1198

preconcentration

in trace analysis

An operation (process) as a result of which the ratio of the concentration or the amount of microcomponents (trace constituents) and macrocomponents (matrix) increases. The term enrichment is not recommended.

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1197

precursor complex

May either indicate an encounter complex or a collision complex, but furthermore implies that this complex undergoes a reaction (e.g. electron transfer).

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

precursor

in radioanalytical chemistry

Of a nuclide, any radioactive nuclide which precedes that nuclide in a decay chain.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523

precursor ion

in mass spectrometry

Synonymous with parent ion.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1549
Orange Book, p. 205

predissociation

Dissociation occurring by tunnelling from a 'bound' to an 'unbound' vibronic state. In an absorption spectrum of a molecular entity, the appearance of a diffuse band region within a series of sharp bands is called predissociation, since irradiation with frequencies within the diffuse region leads to effective dissociation. The energy of the band is smaller than that of the dissociation continuum of the bound state.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

preferential sorption

Synonym: selective sorption *in polymer chemistry*

in polymers

An equilibrium phenomenon, operative in polymer solutions in multicomponent solvents and in polymer networks swollen by multicomponent solvents, that produces differences in solvent composition in the polymer-containing region and in the pure solvent which is in thermodynamic equilibrium with that region. Synonymous with selective sorption.

Source:
Purple Book, p. 59

premium coke

An extremely well graphitizing carbon with a high degree of optical anisotropy (isochromatic areas of optical texture above about $100\ \mu\text{m}$) and which is characterized by a combination of the following properties which differ significantly from those of regular coke: high real density, low reversible thermal expansion and low ash content combined, in most cases, with low sulfur content.
Note:
Premium coke is mainly produced from tars or residues from petrochemistry by the delayed coking process. Also, refined coal tar pitches are used as precursors for premium coke production.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 501

premix burner

in flame spectroscopy

A burner in which fuel and oxidant are thoroughly mixed inside the burner housing before they leave the burner ports and enter the primary-combustion or inner zone of the flame. This type of burner usually produces an approximately laminar flame, and is commonly combined with a separate unit for nebulizing the sample.

Source:
Orange Book, p. 165

prenols

Alcohols possessing the general formula $H–[CH_2C(Me)=CHCH_2]_nOH$ in which the carbon skeleton is composed of one or more isoprene units (biogenetic precursors of the isoprenoids).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1360
White Book, p. 252

prepolymer

Polymer or oligomer the molecules of which are capable of entering, through reactive groups, into further polymerization and thereby contributing more than one structural unit to at least one type of chain of the final polymer.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 897

prepreg

Sheets of a substrate that have been impregnated with a curable polymer, curable polymers, or liquid reactants, or a thermoplastic, and are ready for fabrication of laminates.
Note:
During the impregnation, the curable polymer, curable polymers, or liquid reactants may be allowed to react to a certain extent (sometimes termed degree of ripening).

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1991

pressure, p

Normal force acting on a surface divided by the area of that surface. For a mixture of gases the contribution by each constituent is called the partial pressure $p_i = x_i\,p$, where x_i is the amount fraction of the ith constituent and p is the total pressure.

Source:
Green Book, 2nd ed., p. 12
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 987

pressure gradient correction factor

in gas chromatography

A factor that corrects for the compressibility of the carrier gas. The values of the measured quantities obtained after multiplication by the factor j are independent of the pressure drop in the column. If p_{i}, p_{o} are respectively the pressures of the carrier gas at the inlet and outlet of the column, then j is given by:

$$j = \frac{3\left[\left(\frac{p_{\mathrm{i}}}{p_{\mathrm{o}}}\right)^2 - 1\right]}{2\left[\left(\frac{p_{\mathrm{i}}}{p_{\mathrm{o}}}\right)^3 - 1\right]}$$

Source:
Orange Book, p. 101

pressure jump

See: relaxation

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2297

pressure-induced transition

A transition induced by a change of pressure. Example: The room-temperature transition of CdS with a wurtzite-type structure, at $1.74\ \mathrm{GPa}$, to CdS with a NaCl-type structure.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 589

pressure-sensitive detector

A detector which employs the pressure change which results from the absorption of radiation.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1752

pretreatment

of a catalyst

Following the preparation of a catalyst or following its insertion into a catalytic reactor, it is often subjected to various treatments before the start of a catalytic run. The term pretreatment may, in general, be applied to this set of treatments. In some cases the word activation is used. It implies that the material is converted into a catalyst or into a very much more effective one by the pretreatment.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

primary crystallization

The first stage of crystallization, considered to be ended when most of the spherulite surfaces impinge on each other. In isothermal crystallization, primary crystallization is often described by the Avrami equation.

Source:
Purple Book, p. 85

primary electrons (pe)

in in situ microanalysis

Electrons generated by a thermal or field emission source used to bombard the specimen for generation of the analytical signals.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2026

primary isotope effect

A kinetic isotope effect attributable to isotopic substitution of an atom to which a bond is made or broken in the rate-controlling step or in a pre-equilibrium step of a specified reaction. The corresponding isotope effect on the equilibrium constant of a reaction in which one or more bonds to isotopic atoms are broken, is called a 'primary equilibrium isotope effect'.
See also: secondary isotope effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1130

primary kinetic isotope effect

See: isotope effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1152

primary mixture

A mixture obtained directly from two or more components intended for the preparation of more dilute calibration mixtures (called secondary or tertiary mixtures).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2208

primary pH standards

Certain substances which meet the criteria of:
1. reproducible preparation in a highly pure state;
2. stability of solution over a reasonable period of time;
3. having a low value of the residual liquid junction potential;
4. having pH betwen 3 and 11.

Source:
Orange Book, p. 19

primary photochemical process (primary photoreaction)

Any elementary chemical process undergone by an electronically excited molecular entity and yielding a primary photoproduct.
See: primary (photo)process

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

primary (photo)process [obsolete]

The term primary (photo)process for photophysical processes is apt to lead to inconsistencies, and its use is therefore discouraged.
See: primary photochemical process

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

primary (photo)product

The first observable chemical entity which is produced in the primary photochemical process and which is chemically different from the reactant.

See: primary (photo)process

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

primary pollutant

in atmospheric chemistry

A pollutant emitted directly into the air from identifiable sources (e.g. SO_2, NO, hydrocarbons, etc.). Secondary pollutants, such as ozone, are generated within the atmosphere through chemical changes which occur in primary pollutants.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2208

primary sample

The collection of one or more increments or units initially taken from a population. The portions may be either combined (composited or bulked sample) or kept separate (gross sample). If combined and mixed to homogeneity, it is a blended bulk sample. The term 'bulk sample' is commonly used in the sampling literature as the sample formed by combining increments. The term is ambiguous since it could also mean a sample from a bulk lot and it does not indicate whether the increments or units are kept separate or combined. Such use should be discouraged because less ambiguous alternative terms (composite sample, aggregate sample) are available. 'Lot sample' and 'batch sample' have also been used for this concept, but they are self limiting terms. The use of 'primary' in this sense is not meant to imply the necessity for multistage sampling.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1205

primary structure

In the context of macromolecules such as proteins, constitutional formula, usually abbreviated to a statement of the sequence and if appropriate cross-linking of chains.
See also: secondary structure, tertiary structure, quaternary structure

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2213

See also:
White Book, p. 80

primary structure

of a segment of a polypeptide

The amino acid sequence of the polypeptide chain(s), without regard to spatial arrangement (apart from configuration at the α-carbon atom).
Note:
This definition does not include the positions of disulfide bonds and is therefore not identical with 'covalent structure'.

Source:
White Book, p. 80

primitive change

One of the conceptually simpler molecular changes into which an elementary reaction can be notionally dissected. Such changes include bond rupture, bond formation, internal rotation, change of bond length or bond angle, bond migration, redistribution of charge, etc. The concept of primitive changes is helpful in the detailed verbal description of elementary reactions, but a primitive change does not represent a process that is by itself necessarily observable as a component of an elementary reaction.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1152

principal group

The characteristic group chosen for citation at the end of a name by a suffix or a class name.

Source:
Blue Book (Guide), p. 13

principal ion

in mass spectrometry

A molecular or fragment ion which is made up of the most abundant isotopes of each of its atomic constituents. In the case of compounds that have been artifically isotopically enriched in one or more positions such as $CH_3{}^{13}CH_3$ or CH_2D_2 the principal ion may be defined by treating the heavy isotopes as new atomic species. Thus, in the above two examples, the principal ions would be of masses 31 and 18, respectively.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

principal moments of inertia

Moments of inertia about the principal axes of the molecule chosen so as to make all the products of inertia equal to zero, $I_A \leq I_B \leq I_C$.

Source:
Green Book, 2nd ed., p. 23

principle of least nuclear motion

The hypothesis that, for given reactants, the reactions involving the smallest change in nuclear positions will have the lowest energy of activation. (It is also often simply referred to as principle of least motion.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1134

principle of microscopic reversibility

In a reversible reaction, the mechanism in one direction is exactly the reverse of the mechanism in the other direction. This does not apply to reactions that begin with a photochemical excitation.
See also: chemical reaction, detailed balancing

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1141

prior distribution, P_0

A product state distribution calculated on the basis of some physical model for the reaction. The distribution usually referred to is that of the products at the instant of their formation.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 178

priority

See: CIP priority

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2213

pro-E, pro-Z

One of a pair of identical groups c attached to a double bond (as in abC=Cc_2) is described as *pro-E* if, when it is arbitrarily assigned CIP priority over the other group c, the stereodescriptor of the molecule becomes *E*. The other group c is then described as *pro-Z.*

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2214

pro-R, pro-S

A stereoheterotopic group c (as in tetrahedral $Xabc_2$) is described as *pro-R* if, when it is arbitrarily assigned CIP priority over the other stereoheterotopic group c, the configuration of the thus generated chiral centre is assigned the stereodescriptor *R*. The other group c is then described as *pro-S*. This method for distinguishing between stereoheterotopic groups can be applied to other kinds of prochiral molecular entities or prochiral parts of molecular entities considered on their own.
See: prochirality centre

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2214

probability density, *P*

Product of the wave function and its complex conjugate.

Source:
Green Book, 2nd ed., p. 16

probability, *P*

Number of favourable events divided by the total number of possible events. It is a number between 0 and 1.

Source:
Green Book, 2nd ed., p. 39

probe

in biotechnology

A specific DNA or RNA sequence which has been labelled by radioactivity, fluorescence labels or chemiluminescence labels and which is used to detect complementary sequences by hybridization techniques such as blotting or colony hybridization.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 163

process

A phenomenon by which change takes place in a system. In physiological systems, a process may be chemical, physical or both.

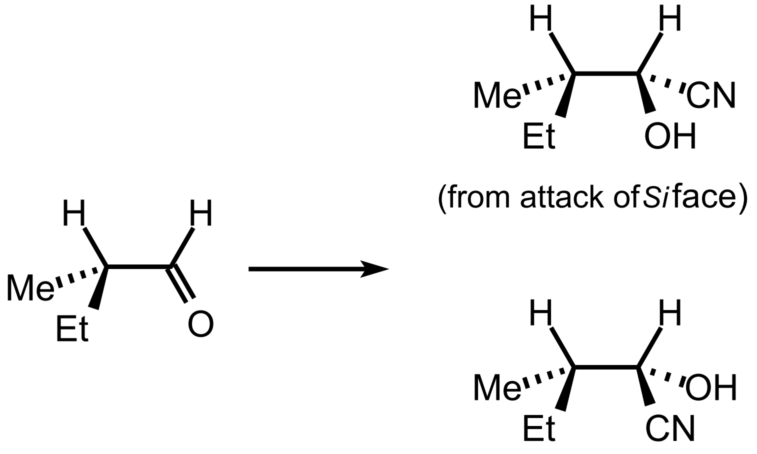
Source:
PAC, 1992, *64*, 1569 *(Quantities and units for metabolic processes as a function of time (IUPAC Recommendations 1992))* on page 1572

prochirality

Also contains definition of: proprochirality

This term is used in different, sometimes contradictory ways; four are listed below.

1. The geometric property of an achiral object (or spatial arrangement of points or atoms) which is capable of becoming chiral in a single desymmetrization step. An achiral molecular entity, or a part of it considered on its own, is thus called prochiral if it can be made chiral by the replacement of an existing atom (or achiral group) by a different one. An achiral object which is capable of becoming chiral in two desymmetrization steps is sometimes described as proprochiral. For example the proprochiral CH_3CO_2H becomes prochiral as CH_2DCO_2H and chiral as $CHDTCO_2H$.
2. The term prochirality also applies to an achiral molecule or entity which contains a trigonal system and which can be made chiral by the addition to the trigonal system of a new atom or achiral group. For example addition of hydrogen to one of the enantiotopic faces of the prochiral ketone $CH_3CH_2COCH_3$ gives one of the enantiomers of the chiral alcohol $CH_3CH_2CHOHCH_3$; the addition of CN^- to one of the diastereotopic faces of the chiral aldehyde shown below converts it into one of the diastereoisomers of the cyanohydrin. The two faces of the trigonal system may be described as *Re* and *Si*.



(from attack of *Si* face)

(from attack of *Re* face)

3. The term prochiral also applies to a tetrahedral atom of an achiral or chiral molecule which is bonded to two stereoheterotopic groups. For example, the prochiral molecule CH_3CH_2OH can be converted into the chiral molecule CH_3CHDOH by the isotopic replacement of one of the two enantiotopic hydrogen atoms of the methylene group. The carbon atom of the methylene group is called prochiral. The prochiral molecule $HO_2CCH_2CHOHCH_2CO_2H$ can be converted into a

chiral product by esterification of one of the two enantiotopic –CH_2CO_2H groups. The carbon atom of the CHOH group is called prochiral. The chiral molecule $CH_3CHOHCH_2CH_3$ can be converted into one of the diastereoisomers of $CH_3CHOHCHDCH_3$ by the isotopic replacement of one of the two diastereotopic hydrogen atoms of the methylene group. The carbon atom of the methylene group is called prochiral. The stereoheterotopic groups in these cases may be described as *pro-R* or *pro-S*. Reference to the two stereoheterotopic groups themselves as prochiral, although common, is strongly discouraged.
See: chirality centre

4. The term prochirality is also applied to the enantiotopic faces of a trigonal system.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2213

prochirality centre

An atom of a molecule which becomes a chirality centre by replacing one of the two stereoheterotopic ligands attached to it by a different ligand, e.g. C-1 of ethanol; C-3 of butan-2-ol.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2214

product

A substance that is formed during a chemical reaction.
See: reactant

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 178

product development control

The term is used for reactions under kinetic control where the selectivity parallels the relative (thermodynamic) stabilities of the products. Product development control is usually associated with a transition state occurring late on the reaction coordinate.
See also: steric-approach control, thermodynamic control

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

product ion

Synonymous with daughter ion.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

product state distribution

The distribution of available energy among the vibrational, rotational and translation degrees of freedom in the product molecules. The distribution usually referred to is that of the products at the instant of their formation.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 178

product-determining step

The step of a stepwise reaction in which the product distribution is determined. The product-determining step may be identical to, or occur later than, the rate-controlling step on the reaction coordinate.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

productivity, r

in biotechnology

An economical figure denoting the mass of a product formed per unit reactor volume and unit time. Productivity is often referred to per unit of enzyme or biomass.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 163

progenitor ion

in mass spectrometry

Synonymous with precursor ion *in mass spectrometry*.

Source:
Orange Book, p. 205

program

Noun: A set of instructions enabling a device to perform an action. Verb: To provide a set of instructions enabling a device to perform an action.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1659

programmed-flow chromatography (flow programming)

A procedure in which the rate of flow of the mobile phase is changed systematically during a part or whole of the separation.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 827

programmed-pressure chromatography (pressure programming)

A procedure in which the inlet pressure of the mobile phase is changed systematically during a part or whole of the separation.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 827

programmed-temperature chromatography (temperature programming)

A procedure in which the temperature of the column is changed systematically during a part or the whole of the separation.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 827

projection formula

Also contains definition of: stereoformula

A formal two-dimensional representation of a three-dimensional molecular structure obtained by projection of bonds (symbolized as lines) onto a plane with or without the designation of the positions of relevant atoms by their chemical symbols. A projection formula which indicates the spatial arrangement of bonds is called a stereochemical formula or stereoformula. Examples of stereoformulae are Fischer projection, Newman projection, sawhorse projection, wedge projection and zig-zag projection.
See also: perspective formula

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2214

prolate trochoidal mass spectrometer

A mass spectrometer in which ions of different mass/charge are separated by means of crossed electric and magnetic fields in such a way that the selected ions follow a prolate trochoidal path. The usual term 'cycloidal' used sometimes is incorrect because the path used is not cycloidal. A cycloid is a special case of a trochoid.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545
Orange Book, p. 203

promoter (gene technology)

The DNA region, usually upsteam to the coding sequence of a gene or operon, which binds and directs RNA polymerase to the correct transcriptional start site and thus permits the initation of transcription.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 163

promoter

in catalysis

A relatively small quantity of one or more substances, which when added to a catalyst improves the activity, the selectivity, or the useful lifetime of the catalyst. In general, a promoter may either augment a desired reaction or suppress an undesired one.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

promotion

See: pseudo-catalysis

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

prompt coincidence

The occurrence of two or more events separated by a time interval which is less than a specified small value.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

prompt neutrons

Neutrons accompanying the fission process without measurable delay.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

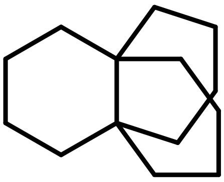
propagation

See: chain reaction

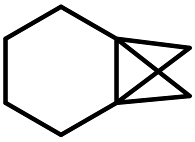
Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

propellanes

Tricyclic saturated hydrocarbons, systematically named tricyclo[$a.b.c.0^{1,(a+2)}$]alkanes; have been referred to as [*a*.*b*.*c*]propellanes.



[4.4.4]propellane



[4.1.1]propellane

See: paddlanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1360

property

A set of data elements (system, component, kind-of-property) common to a set of particular properties, e.g. substance concentration of glucose in blood plasma. Information about identification, time and result is not considered.
See also: particular property

Source:
PAC, 1995, *67*, 1563 *(Properties and units in the clinical laboratory sciences-I. Syntax and semantic rules (IUPAC-IFCC Recommendations 1995))* on page 1565

prophage

The latent state of a phage genome in a lysogenic bacterium.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 163

proportional counter

A gas-filled X-ray detector in which the electric potential is high enough for the gain to reach a value in the range from 10^2 to 10^5. Each electron produced by the initial photo-ionization causes one avalanche. Since the number of avalanche events is proportional to the energy of the incident photons, the charge collected by the anode is proportional to the X-ray photon energy.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1754

proportional counter tube

A counter tube operated under such conditions that the magnitude of each pulse is proportional to the amount of energy deposited in it.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

proportional gas-scintillation counter

A proportional counter coupled to an ultraviolet sensitive photomultiplier tube. Initial electrons produced by the interaction of the high-energy photon with the counter fill-gas are accelerated by a high electric field where they acquire sufficient energy to excite the noble gas atoms. The resulting UV radiation is observed by a photomultiplier tube.

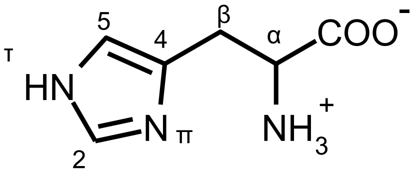
Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1754

pros

Also contains definition of: *tele in histidine nomenclature*

in histidine nomenclature

The nitrogen atoms of the imidazole ring of histidine are denoted by *pros* ('near', abbreviated π) and *tele* ('far', abbreviated τ) to show their position relative to the side chain. This recommendation arose from the fact that two different systems of numbering the atoms in the imidazole ring of histidine had both been used for a considerable time (biochemists generally numbering as 1 the nitrogen atom adjacent to the side chain, and organic chemists designating it as 3). The carbon atom between the two ring nitrogen atoms is numbered 2 (as in imidazole), and the carbon atom next to the τ nitrogen is numbered 5. The carbon atoms of the aliphatic chain are designated α and β. This numbering should also be used for the decarboxylation product histamine and for substituted histidine.

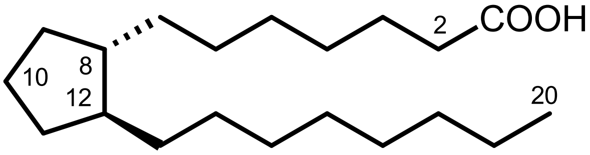


histidine

Source:
White Book, p. 43

prostaglandins

Naturally occurring compounds derived from the parent C_{20} acid, prostanoic acid.



See: icosanoids, prostanoids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1360

prostanoids

The family of natural prostaglandins and prostaglandin-like compounds.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1360

prosthetic group

The non-amino acid portion of a conjugated protein. Examples include cofactors such as flavines or cytochromes as well as lipids and polysaccharides, which are the prosthetic groups of lipoproteins and glycoproteins, respectively.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 163

proteases

Enzymes that catalyse the hydrolysis of proteins. Usually several proteolytic enzymes are necessary for the complete breakdown of polypeptides to their amino acids.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 163

protected lyophobic colloid

A colloidally stable mixture of a lyophobic and a lyophilic colloid.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

protection of a reactive group

Temporary chemical transformation of a reactive group into a group that does not react under conditions where the non-protected group reacts.
Note:
For example, trimethylsilylation is a typical transformation used to protect reactive functional groups, such as hydroxy or amino groups, from their reaction with growing anionic species in anionic polymerization.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 894

protective action

in colloid chemistry

Addition of small amounts of hydrophilic colloid to a hydrophobic sol may make the latter more sensitive to flocculation by electrolyte. Higher concentrations of the same hydrophilic colloid usually protect the hydrophobic sol from flocculation. This phenomenon is called protective action.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

protein engineering

A technique used to produce proteins with altered or novel amino acid sequences. The methods used are:

1. Transcription and translation systems from synthesized lengths of DNA or RNA with novel sequences.
2. Chemical modification of 'normal' proteins.

3. Solid-state polypeptide synthesis to form proteins.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 163

proteins

Naturally occurring and synthetic polypeptides having molecular weights greater than about 10000 (the limit is not precise).
See also: peptides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

See also:
White Book, p. 48

proteoglycan

A subclass of protein in which the carbohydrate units are polysaccharides that contain amino sugars. The protein is glycosylated by one or more (up to about 100) glycosaminoglycans [linear polymers of up to about 200 repeating disaccharide units that consist of a hexosamine (D-glucosamine or D-galactosamine) alternating with a uronic acid (D-glucuronic or L-iduronic) or a neutral sugar (D-galactose)].

Source:
PAC, 1988, *60*, 1389 *(Nomenclature of glycoproteins, glycopeptides and peptidoglycans (Recommendations 1985))* on page 1391
White Book, p. 85

proteome

Complete set of proteins encoded by the genome.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1066

protic

See: protogenic

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

protium

Also contains definitions of: protide, protio

A specific name for the atom ^1H. The cation $^1H^+$ is a proton, the species ^1H is a protide anion, and ^1H is the protio group. The word proton should not be used for H^+ in its natural abundance.

Source:
PAC, 1988, *60*, 1115 *(Names for hydrogen atoms, ions, and groups, and for reactions involving them (Recommendations 1988))* on page 1116

protogenic (solvent)

Capable of acting as a proton donor (strongly or weakly acidic as a Brønsted acid). The term is preferred to the synonym protic or the more ambiguous expression acidic by itself.

Source:
PAC, 1983, *55*, 1281 *(Glossary of terms used in physical organic chemistry)* on page 1348

protolysis **[obsolete]**

This term has been used synonymously with proton (hydron)-transfer reaction. Because of its misleading similarity to hydrolysis, photolysis, etc., its use is discouraged.
See also: autoprotolysis

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

proton

Nuclear particle of charge number $+1$, spin quantum number $\frac{1}{2}$ and rest mass of $1.007\ 276\ 470(12)\ \mathrm{u}$.
See also: protium

Source:
Green Book, 2nd ed., p. 93

proton affinity

The negative of the enthalpy change in the gas phase reaction (real or hypothetical) between a proton (more appropriately hydron) and the chemical species concerned, usually an electrically neutral species to give the conjugate acid of that species. Proton affinity is often, but unofficially, abbreviated as PA.
See also: gas phase basicity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

proton magnetic moment

Atomic fundamental physical constant $\mu_{\mathrm{p}} = 1.410\,607\,61(47) \times 10^{-26}\ \mathrm{J\ T^{-1}}$.

Source:
CODATA Bull. 1986, *63*, 1

proton magnetogyric ratio

Atomic fundamental physical constant $\gamma_{\mathrm{p}} = 2.675\,221\,28(81) \times 10^{8}\ \mathrm{s^{-1}\ T^{-1}}$.

Source:
CODATA Bull. 1986, *63*, 1

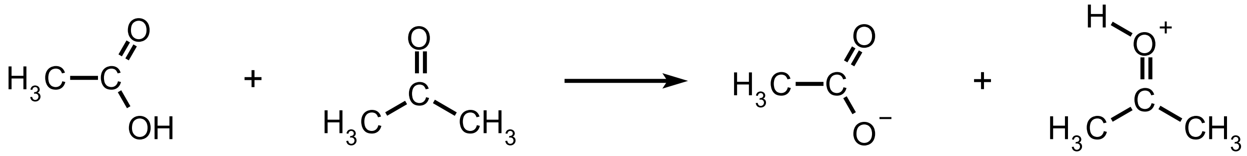
proton rest mass

Atomic fundamental physical constant $m_{\mathrm{p}} = 1.672\,6231(10) \times 10^{-27}\ \mathrm{kg}$.

Source:
CODATA Bull. 1986, *63*, 1

proton transfer reaction

A chemical reaction, the main feature of which is the intermolecular or intramolecular transfer of a proton (hydron) from one binding site to another. For example:



In the detailed description of proton transfer reactions, especially of rapid proton transfers between electronegative atoms, it should always be specified whether the term is used to refer to the overall process (including the more-or-less encounter-controlled formation of a hydrogen bonded complex and the separation of the products; see microscopic diffusion control) or just to the proton transfer event (including solvent rearrangement) by itself.
See also: autoprotolysis, tautomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

protonated molecule

in mass spectrometry

An ion formed by interaction of a molecule with a proton abstracted from an ion, as often occurs in chemical ionization according to the reaction: $M + XH^+ \rightarrow MH^+ + X$. The symbolism $[M + H]^+$ may also be used to represent the protonated molecule. The widely used term 'protonated molecular ion' to describe the MH^+ ion is not recommended, since it suggests an associated product of a proton with a molecular ion.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

protonation constant

The equilibrium constant K_{Hn} for the addition of the nth proton to a charged or uncharged ligand. The cumulative protonation constant, β_{Hn}, is the equilibrium constant for the formation of H_nL from nH^+ and L. The same equilibrium constant may be described in several ways, depending on how the ligand, L, or the acid, has been defined.

Source:
Orange Book, p. 13

protophilic (solvent)

Capable of acting as proton acceptor, strongly or weakly basic (as a Brønsted base). Also called HBA (hydrogen bond acceptor) solvent.
See also: protogenic solvent

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

protoplast

A spherical, osmotically-sensitive cell without its cell wall but retaining an intact cell membrane. Protoplasts are used to create hybrid cells via protoplast fusion.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 164

prototrophs

Microoganisms capable of growing at or below a temperature optimum of 15 °C.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 164

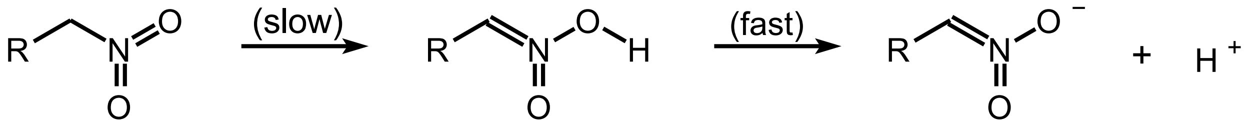
prototropic rearrangement (or prototropy)

See: tautomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

pseudo acids

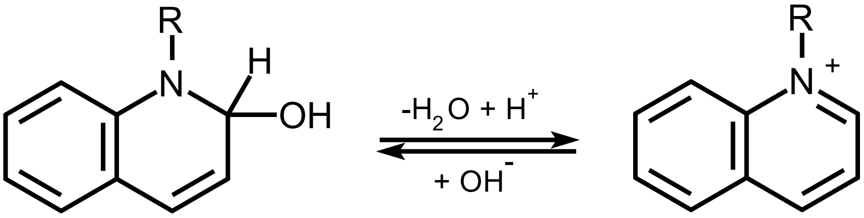
Potentially acidic compounds that require some structural reorganization, such as keto–enol tautomerization, having a non-negligible activation energy, in order to show normal acidic properties, e.g. nitroalkanes:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

pseudo bases

Hydroxy compounds that give salts with acids by formation of water accompanied by a change of constitution.



See: anhydro bases

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

pseudo rate constant

A term sometimes used for a rate coefficient. For example, if the rate equation is:

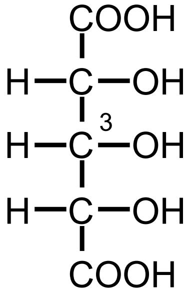
$v = k\ [\mathrm{A}]\ [\mathrm{B}]$

the function $k\ [\mathrm{A}]$ is the pseudo first-order rate constant (or first-order rate coefficient) with respect to B. Similarly, $k\ [\mathrm{B}]$ is the pseudo first-order rate constant (or first-order rate coefficient) with respect to A. The term pseudo rate constant is particularly useful when the concentration of one reactant is much greater than that of another.
See also: rate coefficient

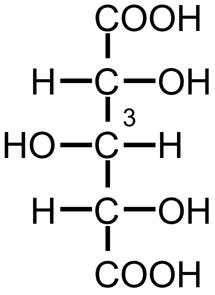
Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 178

pseudo-asymmetric carbon atom

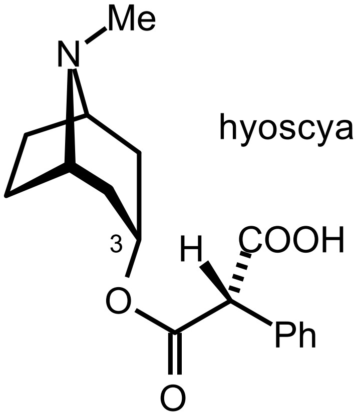
The traditional name for a tetrahedrally coordinated carbon atom bonded to four different entities, two and only two of which have the same constitution but opposite chirality sense. The *r/s* descriptors of pseudo-asymmetric carbon atoms are invariant on reflection in a mirror (i.e. *r* remains *r*, and *s* remains *s*), but are reversed by the exchange of any two entities (i.e. *r* becomes *s*, and *s* becomes *r*). An example is C-3 of ribaric (C-3 is *r*) or xylaric acid (C-3 is *s*) or hyoscyamine (C-3 is *r*). The hyphen in pseudo-asymmetric may be omitted.



ribaric acid



xylaric acid



hyoscyamine

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2214

pseudo-catalysis

If an acid or base is present in nearly constant concentration throughout a reaction in solution (owing to buffering or the use of a large excess), it may be found to increase the rate of that reaction and also to be consumed during the process. The acid or base is then not a catalyst and the phenomenon cannot be called catalysis according to the well-established meaning of these terms in chemical kinetics, although the mechanism of such a process is often intimately related to that of a catalysed reaction. It is recommended that the term pseudo-catalysis be used in these and analogous cases (not necessarily involving acids or bases). For example, if a Brønsted acid accelerates the hydrolysis of an ester to a carboxylic acid and an alcohol, this is properly called acid catalysis, whereas the acceleration, by the same acid, of hydrolysis of an amide should be described as pseudo-catalysis by the acid: the 'acid pseudo-catalyst' is consumed during the reaction through formation of an ammonium ion. The terms 'general acid pseudo-catalysis' and 'general base pseudo-catalysis' may be used as the analogues of general acid catalysis and general base catalysis. The term 'base-promoted', 'base-accelerated' or 'base-induced' is sometimes used for reactions that are pseudo-catalysed by bases. However, the term 'promotion' also has a different meaning in other chemical contexts.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1153

pseudo-co-oligomer

An irregular oligomer, the molecules of which are derived from only one species of monomer but which display a variety of structural features more appropriate for description in co-oligomer terms.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2300

pseudo-copolymer

Also contains definition of: statistical pseudo-copolymer

An irregular polymer, the molecules of which are derived from only one species of monomer but which display a variety of structural features more appropriate for description in copolymer terms.
Note:
Where appropriate, adjectives specifying the types of 'copolymer' may be applied to 'pseudo-copolymer'. The term statistical pseudo-copolymer, for instance, may be used to describe an irregular polymer in the molecules of which the sequential distribution of configurational units obeys known statistical laws.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2300

pseudo-first-order reaction

See: order of reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1154

pseudo-unimolecular [obsolete]

A term sometimes used as synonymous with pseudo-first-order, but is inherently meaningless.
See: molecularity, order of reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1154

pseudo-zero-order reaction

See: order of reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1154

pseudohalogens

Compounds that resemble the halogen elements, X_2, in their chemistry, e.g. $(CN)_2$ cyanogen, $(SCN)_2$ thiocyanogen, ICN iodine cyanide. Certain ions that have sufficient resemblance to halide ions are sometimes referred to as pseudohalide ions, e.g. N_3^-, SCN^-, CN^-.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

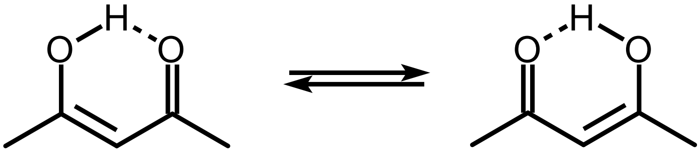
pseudomolecular rearrangement [obsolete]

The use of this awkwardly formed term is discouraged. It is synonymous with 'intermolecular rearrangement'.
See: molecular rearrangement

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1154

pseudopericyclic

A concerted transformation is pseudopericyclic if the primary changes in bonding occur within a cyclic array of atoms at one (or more) of which nonbonding and bonding atomic orbitals interchange roles. A formal example is the enol → enol prototropy of pentane-2,4-dione (acetylacetone).



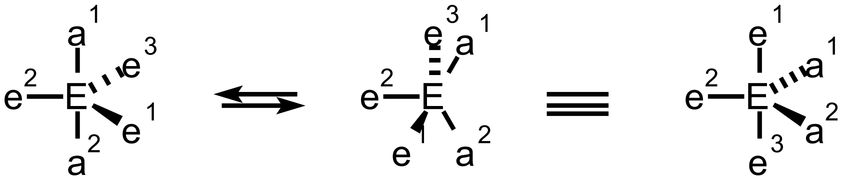
Because the π- and σ-atomic orbitals that interchange roles are orthogonal, such a reaction does not proceed through a fully conjugated transition state and is thus not a pericyclic reaction and therefore not governed by the rules that express orbital symmetry restrictions applicable to pericyclic reactions.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1154

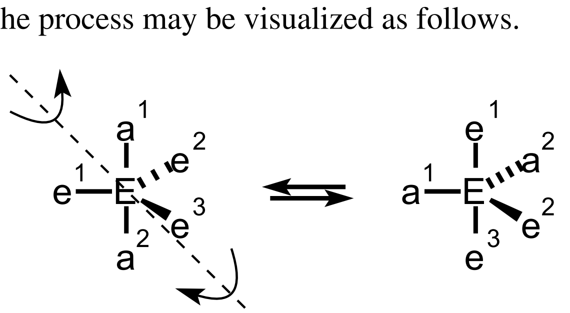
pseudorotation

Also contains definitions of: Berry pseudorotation, turnstile rotation

Stereoisomerization resulting in a structure that appears to have been produced by rotation of the entire initial molecule and is superposable on the initial one, unless different positions are distinguished by substitution, including isotopic substitution. One example of pseudorotation is a facile interconversion between the many envelope and twist conformers of a cyclopentane due to the out of plane motion of carbon atoms. Another example of pseudorotation (Berry pseudorotation) is a polytopal rearrangement that provides an intramolecular mechanism for the isomerization of trigonal bipyramidal compounds (e.g. λ^5-phosphanes), the five bonds to the central atom E being represented as e^1, e^2, e^3, a^1 and a^2. Two equatorial bonds move apart and become apical bonds at the same time as the apical bonds move together to become equatorial.



A related conformational change of a trigonal bipyramidal structure is described as turnstile rotation. The process may be visualized as follows.



An apical and an equatorial bond rotate as a pair ca. 120° relative to the other three bonds. (Doubts have been expressed about the distinct physical reality of this mechanism.)

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2215

pseudoureas [obsolete]

An obsolescent synonym for isoureas.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

psychosine

See: glycolipids

Source:
White Book, p. 129

psychrometric hygrometer

Instrument by which the relative humidity of the atmosphere may be determined. It is generally composed of two temperature sensors, one of which measures the temperature of the air; the other sensor is moistened with water and senses the cooling due to evaporation of water. The temperature difference between the two sensors is a function of relative humidity; sometimes referred to as a 'wet-and-dry bulb' thermometer.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2196

psychrometry

The use of a wet-and-dry bulb thermometer for measurement of atmospheric humidity.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2208

puffing

An irreversible expansion of some carbon artifacts during graphitization heat treatment between 1650 and $2700\ \mathrm{K}$.
Note:

Puffing is caused by the release of heteroatoms, for instance sulfur atoms, from the coke in association with specific microstructural rearrangements.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 502

puffing inhibitor

Metals or metal compounds with a high chemical affinity for the heteroatoms in the carbons. They are distributed as fine particles within the carbon materials to be graphitized.
Note:
Iron and iron compounds are most frequently used as puffing inhibitors when puffing is related to sulfur.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 502

pulse amplitude analyser

Synonym: pulse height analyser

A sub-assembly for determining the distribution function of a set of pulses in terms of their amplitude. Synonymous with pulse height analyser.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

pulse amplitude selector

Synonym: single channel pulse height analyser

A circuit which gives an output pulse for each input pulse whose amplitude lies within a chosen interval. Synonymous with single channel pulse height analyser.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1548

pulse duration

in electroanalytical chemistry

In pulse polarography, differential pulse polarography, Kalousek polarography, and related techniques, the duration of an interval during which the excitation signal deviates from the base line. This interval includes the sampling interval.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1503

pulse reactor

in catalysis

In a pulse reactor, a carrier gas, which may be inert or possibly one of the reactants, flows over the catalyst and small amounts of the other reactant or reactants are injected into the carrier gas at intervals. A pulse reactor is useful for exploratory work but kinetic results apply to a transient rather than to the steady state conditions of the catalyst.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

pump-dump-probe technique

Transient absorption spectroscopy using three pulses (a strong pump, a dump pulse that can alter the course of the reaction photoinduced by the first pulse, and a weak probe). In general, femtosecond laser pulses are used.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 404

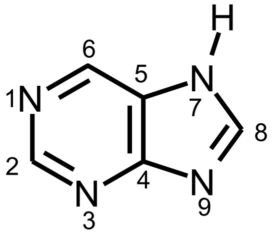
pump-probe technique

Transient absorption spectroscopy using two pulses (strong pump and weak probe) and capable of achieving a high temporal resolution. A pump pulse excites the sample and triggers the process under investigation. A second delayed pulse, the probe, monitors an optical property. By varying the time delay between the pump and probe pulses, it is possible to assemble measurements as a function of time. The probe pulse is typically a UV, visible or infrared pulse in which case a snap-shot spectrum is taken as a function of the delay time. Often the probe pulse is generated from a portion of the excitation beam, but it can also be an independently generated electromagnetic pulse.
Note:
In the case of an optical probe, this interaction is formally a non-linear optical process that is third-order in polarization. The excitation intensity to create the excited state constitutes a two-field interaction and the determination of the change in the time-dependent optical properties involves a third field monitoring the induced time-dependent changes in the 'linear susceptibility'. Diffractive probes (e.g., electrons and X-rays) can also be used, in which case one measures a diffraction pattern as a function of time.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 404

purine bases

Purine and its substitution derivatives, especially naturally occurring examples. The customary numbering shown below is not systematic.

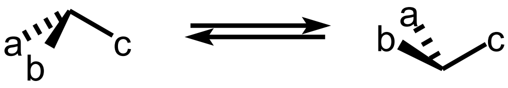


purine

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

pyramidal inversion

A polytopal rearrangement in which the change in bond directions to a three-coordinate central atom having a pyramidal arrangement of bonds (tripodal arrangement) causes the central atom (apex of the pyramid) to appear to move to an equivalent position on the other side of the base of the pyramid. If the three ligands to the central atom are different pyramidal inversion interconverts enantiomers.



Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2215

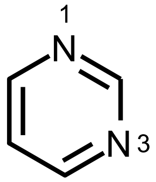
pyranoses

Cyclic hemiacetal forms of monosaccharides in which the ring is six-membered (a tetrahydropyran).
See: furanoses

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

pyrimidine bases

Pyrimidine and its substitution derivatives, especially naturally occurring examples.



pyrimidine

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

pyro

A prefix designating compounds formed by heating a compound, usually with the elimination of water, carbon dioxide, or other simple molecule, e.g. pyroglutamic acid from glutamic acid.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

pyroelectric detector

A detector (based on the temperature dependence of ferroelectricity in some crystals) which produces an electrical signal proportional to the energy flux on the collector surface.

Source:
Orange Book, p. 193

See also:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1752

pyrolysis

Thermolysis, usually associated with exposure to a high temperature.
Notes:

1. The term generally refers to reaction in an inert environment.
2. Pyrolysis is the commonly used term for a high-temperature treatment that converts a ceramic precursor to a ceramic.
3. Modified from previous definition. The definition proposed here is more explicit about the elevated temperatures involved.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1824

pyrolysis-gas chromatography

A version of reaction chromatography in which a sample is thermally decomposed to simpler fragments before entering the column.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 827

pyrolytic carbon

A carbon material deposited from gaseous hydrocarbon compounds on suitable underlying substrates (carbon materials, metals, ceramics) at temperatures ranging from 1000 to $2500\ \mathrm{K}$ (chemical vapour deposition).
Note:
A wide range of microstructures, e.g. isotropic, lamellar, substrate-nucleated and a varied content of remaining hydrogen, can occur in pyrolytic carbons, depending on the deposition conditions (temperature, type, concentration and flow rate of the source gas, surface area of the underlying substrate, etc.). 'Pyrocarbon' which is synonymous with pyrolytic carbon was introduced as a trademark and should not be used as a term. The term pyrolytic carbon does not describe the large range of carbon materials obtained by thermal degradation (thermolysis, pyrolysis) of organic compounds when they are not formed by chemical vapour deposition (CVD). Also, carbon materials, obtained by physical vapour deposition (PVD) are not covered by the term pyrolytic carbon.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 502

pyrolytic graphite

A graphite material with a high degree of preferred crystallographic orientation of the *c*-axes perpendicular to the surface of the substrate, obtained by graphitization heat treatment of pyrolytic carbon or by chemical vapour deposition at temperatures above $2500\ \mathrm{K}$.
Note:
'Pyrographite', a synonym for pyrolytic graphite, was introduced as a trademark and should not be used as a term. Hot working of pyrolytic graphite (by heat treatment under compressive stress at temperatures above $3000\ \mathrm{K}$) results in highly oriented pyrolytic graphite (HOPG).

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 502

pyrromethenes

A less preferred term for dipyrrins. (The term 'pyrromethane' has been used for the system with a $-CH_2-$ linkage).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

Q-switched laser

A laser in which the state of the device introducing important losses in the resonant cavity and preventing lasing operation is suddenly switched to a state where the device introduces very low losses. This increases rapidly the Quality factor of the cavity, allowing the build-up of a short and very intense laser pulse. Typical pulse durations are in the ns range. The Q-switching may be active (a rotating mirror or electro-optic device) or passive (a saturable absorber).
See also: free-running laser

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2266

quadratic mean, $\bar{x}_\mathrm{q}$

The square root of the expression in which the sum of squared observations is divided by the number n. It can be calculated by the formula:

$$\bar{x}_\mathrm{q} = \sqrt{\frac{\sum x_i^2}{n}}$$

Comment:
This quantity is also sometimes directly (but inappropriately) calculated, for example, when an observable is proportional to the square of concentration. The quadratic mean, also known as the root mean square, is sometimes appropriate, however, as in certain of the formulae connected with linear calibration functions.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 602

quadro-

An affix used in names to denote four atoms bound into a quadrangle (e.g. square).

Source:
Red Book, p. 245
Blue Book, p. 465

quadrupole ion storage trap (Quistor)

An arrangement in which ions with a desired range of quotients mass/charge are trapped by making them describe stable paths under the effect of a static and a high-frequency electric quadrupole field.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

quadrupole mass analyser

An arrangement in which ions with a desired quotient mass/charge are made to describe a stable path under the effect of a static and a high-frequency electric quadrupole field, and are then detected. Ions with a different mass/charge are separated from the detected ions because of their unstable paths.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1545
Orange Book, p. 202

quadrupole splitting

in Mössbauer spectroscopy

The measured Doppler velocity difference between the two peaks seen in quadrupole split spectra from nuclides such as ^{57}Fe and ^{119}Sn.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 214

qualitative analysis

Analysis in which substances are identified or classified on the basis of their chemical or physical properties, such as chemical reactivity, solubility, molecular weight, melting point, radiative properties (emission, absorption), mass spectra, nuclear half-life, etc.
See also: quantitative analysis

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1701

qualitative elemental specificity

in analysis

Ability of a method to detect one element in the presence of another element.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

quality assurance

The guarantee that the quality of a product (analytical data set, etc.) is actually what is claimed on the basis of the quality control applied in creating that product. Quality assurance is not synonymous with quality control. Quality assurance is meant to protect against failures of quality control.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2208

quality control

The maintenance and statement of the quality of a product (data set, etc.) specifically that it meets or exceeds some minimum standard based on known, testable criteria.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2208

quality factor

in nuclear analytical chemistry

The linear-energy-transfer dependent factor by which absorbed dose is multiplied to obtain dose equivalent.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1549

quality of solvent

in polymer chemistry

A qualitative characterization of the polymer–solvent interaction. A solution of a polymer in a 'better' solvent is characterized by a higher value of the second virial coefficient than a solution of the same polymer in a 'poorer' solvent.

Source:
Purple Book, p. 57

quantitative analysis

Analyses in which the amount or concentration of an analyte may be determined (estimated) and expressed as a numerical value in appropriate units. Qualitative analysis may take place without quantitative analysis, but quantitative analysis requires the identification (qualification) of the analytes for which numerical estimates are given.

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1701

quantitative structure–activity relationship (QSAR)

in drug design

Quantitative structure–activity relationships (QSAR) are mathematical relationships linking chemical structure and pharmacological activity in a quantitative manner for a series of compounds. Methods which can be used in QSAR include various regression and pattern recognition techniques.
QSAR is often taken to be equivalent to chemometrics or multivariate statistical data analysis. It is sometimes used in a more limited sense as equivalent to Hansch analysis. QSAR is a subset of the more general term SPC.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1149

quantitative structure–activity relationships (QSAR)

The building of structure–biological activity models by using regression analysis with physicochemical constants, indicator variables or theoretical calculations. The term has been extended by some authors to include chemical reactivity, i.e. activity is regarded as synonymous with reactivity. This extension is, however, discouraged.
See also: correlation analysis

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1155

quantity

Attribute of a phenomenon, body or substance that may be distinguished qualitatively and determined quantitatively.
Notes:

1. The term quantity may refer to a quantity in a general sense, for example length, mass, or to a particular quantity, for example length of a particular rod, mass of a specified object.
2. The term kind-of-quantity refers to the abstract concept of a quantity common to a group of related quantities.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 987

quantity calculus

Algebra with quantities where the symbols of quantities represent products of numerical values and their units.

Source:
Green Book, 2nd ed., p. 3

quantity of dimension one (dimensionless quantity)

Quantity in the dimensional expression of which all the exponents of the dimensions of the base quantities are zero.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 987

quantized internal energy

The quantized internal energy of a molecule in its electronic ground or excited state can be approximated with sufficient accuracy for analytical purposes by:

$$E_{\mathrm{int}} = E_{\mathrm{el}} + E_{\mathrm{vib}} + E_{\mathrm{rot}}$$

where E_{el} is the electronic, E_{vib} the vibrational and E_{rot} the rotational energy, respectively.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1452

quantum counter

A medium emitting with a quantum yield independent of the excitation energy over a defined spectral range (e.g, concentrated rhodamine 6G solutions between 300 and $600\ \mathrm{nm}$). Also used for devices producing an electrical signal proportional to the photon flux absorbed in a medium.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2267
Orange Book, p. 193
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 238

quantum efficiency

See: efficiency
For a primary photochemical process, quantum efficiency is identical to quantum yield.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2267

quantum mechanics/molecular mechanics

Acronym: QM/MM

Also contains definition of: QC/MM

Hybrid procedure for the treatment of large molecular systems. A crucial part of the system (e.g., the chromophore and its surroundings) is treated explicitly by quantum mechanical (QM) techniques, whereas the rest of the system is approximated by a classical or molecular mechanics (MM) force field treatment.
Note:
Sometimes called QC/MM.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 406

quantum

of radiation

An elementary particle of electromagnetic energy in the sense of the wave-particle duality.
See: photon

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2267

quantum yield, Φ

Number of defined events occurring per photon absorbed by the system.
The integral quantum yield is

$$\Phi(\lambda) = \frac{\text{number of events}}{\text{number of photons absorbed}}$$

For a photochemical reaction,

$$\Phi(\lambda) = \frac{\text{amount of reactant consumed or product formed}}{\text{amount of photons absorbed}}$$

The differential quantum yield is

$$\Phi(\lambda) = \frac{\mathrm{d}x / \mathrm{d}t}{q_{n,\mathrm{p}}^{0}\,[1 - 10^{-A(\lambda)}]}$$

where $\mathrm{d}x / \mathrm{d}t$ is the rate of change of a measurable quantity (spectral or any other property), and $q_{n,\mathrm{p}}^{0}$ the amount of photons (mol or its equivalent einstein) incident (prior to absorption) per time interval (photon flux, amount basis). $A(\lambda)$ is the absorbance at the excitation wavelength.
Notes:

1. Strictly, the term quantum yield applies only for monochromatic excitation. Thus, for the differential quantum yield, the absorbed spectral photon flux density (number basis or amount basis) should be used in the denominator of the equation above when x is either the number concentration ($C = N / V$), or the amount concentration (c), respectively.
2. Φ can be used for photophysical processes (such as, e.g., intersystem crossing, fluorescence and phosphorescence) or photochemical reactions.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 406

quantum-mechanical tunnelling

See: tunnelling

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 178

quarter-transition-time potential

In chronopotentiometry (at constant current density), the potential of the indicator electrode at the instant when the time that has elapsed since the application of current is equal to one-fourth of the transition time. Appropriate correction for double-layer charging is needed in practice.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1502

quartet state

A state having a total electron spin quantum number equal to $\frac{3}{2}$.
See: multiplicity

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2267

quartz–iodine lamp

Wolfram (tungsten) filament high-intensity incandescent lamp containing iodine in a quartz envelope. Used primarily as a source of visible radiation.
Notes:

1. In halogen lamps, the quartz envelope is closer to the filament than the glass used in conventional light bulbs. Heating the filament to a high temperature causes the tungsten (wolfram) atoms to evaporate and combine with the halogen gas. These heavier molecules are then deposited back on the filament surface. This recycling process increases the life of the tungsten (wolfram) filament

and enables the lamp to produce more light per unit of input energy. Consequently, halogen lamps are used in a variety of applications, including automobile headlights.

2. Halogens other than iodine may be used in these lamps.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 407

quasi-classical trajectory (QCT) method

A procedure for calculating trajectories in which the quantization of the reactants is taken into account, but in which the course of the reaction is treated classically.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 179

quasi-enantiomers

Constitutionally different yet closely related chemical species MX and MY having the opposite chirality sense of the large common chiral moiety M. For example (*R*)-2-bromobutane is a quasi-enantiomer of (*S*)-2-chlorobutane.
See also: quasi-racemic compound

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2215

quasi-equilibrium

In conventional transition-state theory it is assumed that activated complexes are formed in a state of equilibrium with the reactants. They are not in classical equilibrium with the reactants; if they were, addition of more activated complexes to the system would cause the equilibrium to shift in favour of the reactants. This would not occur for an activated complex, and the term quasi-equilibrium is used to denote this special type of equilibrium.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 179

quasi-molecular ion

in mass spectrometry

A protonated molecule or an ion formed from a molecular ion by loss of a hydrogen atom. The use of the term 'pseudo-molecular ion' is not recommended.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

quasi-racemic compound

The crystalline product of a 1:1 association between quasi-enantiomers.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

quasi-single-strand polymer

A regular linear polymer that can be described by a preferred constitutional repeating unit in which only one terminal constituent subunit is connected through a single atom to the other identical constitutional repeating units or to an end group.

Source:
Purple Book, p. 110

quaternary ammonium compounds

Derivatives of ammonium compounds, $(NH_4{}^+)Y^-$, in which all four of the hydrogens bonded to nitrogen have been replaced with hydrocarbyl groups. Compounds having a carbon-nitrogen double bond (i.e. $R_2C{=}N^+R_2Y^-$) are more accurately called iminium compounds. e.g. $[(CH_3)_4N]^+OH^-$, tetramethylammonium hydroxide.
See: onium compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1361

quaternary structure

The defined organization of two or more macromolecules with tertiary structure such as a protein that are held together by hydrogen bonds and van der Waals and coulombic forces.
See also: primary structure, secondary structure, tertiary structure

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

See also:
White Book, p. 80

quencher

A molecular entity that deactivates (quenches) an excited state of another molecular entity, either by energy transfer, electron transfer, or by a chemical mechanism.
See: quenching, Stern–Volmer kinetic relationships

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2268

quenching

Also contains definitions of: dynamic quenching, static quenching

Deactivation of an excited molecular entity intermolecularly by an external environmental influence (such as a quencher) or intramolecularly by a substituent through a non-radiative process.
Notes:

1. When the external environmental influence (quencher) interferes with the behaviour of the excited state after its formation, the process is referred to as dynamic quenching. Common mechanisms include energy transfer, electron transfer, etc.
2. When the environmental influence inhibits the excited state formation the process is referred to as static quenching.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 407

quenching constant

in photochemistry

See: quencher, quenching, Stern–Volmer kinetic relationships

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2268

quenching correction

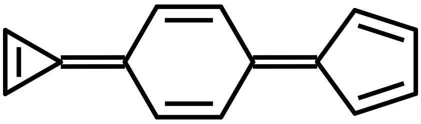
in photochemistry

Correction for errors due to different quenching for standards and test portions. When using liquid scintillation detectors these corrections can be based e.g on the standard addition or sample channels ratio method or the use of automated external standardization.

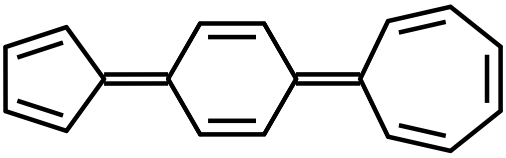
Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523

quinarenes

Mancude assemblies of three carbocyclic rings, a six-membered quinonoid ring bonded at the 1,4-positions to odd-membered rings which differ in ring size by two, e.g.



[3.6.5]quinarene

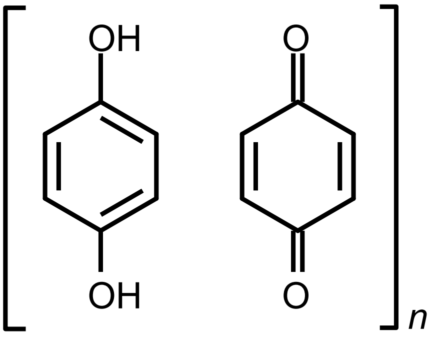


[5.6.7]quinarene

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1362

quinhydrones

Molecular complexes of one equivalent amount of a quinone with one equivalent amount of the corresponding hydroquinone.

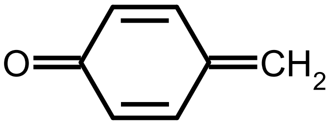


Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1362

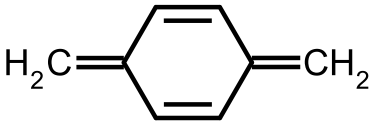
quinomethanes

Also contains definition of: xylylenes

Methylidenecyclohexadienones and dimethylidenecyclohexadienes, formally derived from quinones by replacement of one or both of the quinone oxygens by methylidene groups. (The diradical, triplet state of quinodimethanes can also be called *o*- or *p*-xylylenes).



p-quinomethane



p-quinodimethane

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1362

quinomethides (quinone methides) [obsolete]

Undesirable names for quinomethanes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1362

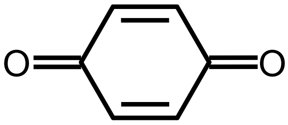
quinone diazides

A potentially confusing term for diazooxides; the presence of an azido group, $-N_3$, is falsely suggested.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1362

quinones

Compounds having a fully conjugated cyclic dione structure, such as that of benzoquinones, derived from aromatic compounds by conversion of an even number of number of –CH= groups into –C(=O)– groups with any necessary rearrangement of double bonds (polycyclic and heterocyclic analogues are included).

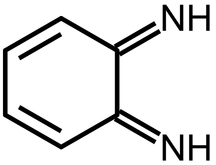


p-benzoquinone

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1362

quinonimines (quinone imines)

Imines derived from quinones by replacement of one or both oxygens by =NR . The term may include both types unless the infix mono or di is included, e.g. *o*-benzoquinone diimine:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1362

quinonoximes

Mono- or di-oximes of quinones; quinone monooximes are tautomeric with nitrosophenols.
See: oximes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1362

ρ-value (rho-value)

A measure of the susceptibility to the influence of substituent groups on the rate constant or equilibrium constant of a particular organic reaction involving a family of related substrates. Defined by Hammett for the effect of ring substituents in *meta*- and *para*-positions of aromatic side-chain reactions by the empirical '$\rho\sigma$-equation' of the general form:

$$\log_{10}\left(\frac{k_{\mathrm{X}}}{k_{\mathrm{H}}}\right) = \rho\,\sigma_{\mathrm{X}}$$

in which σ_{X} is a constant characteristic of the substituent X and of its position in the reactant molecule. More generally (and not only for aromatic series), ρ-values (modified with appropriate subscripts and

superscripts) are used to designate the susceptibility of reaction series for families of various organic compounds to any substituent effects, as given by the modified set of σ-constants in an empirical $\rho\sigma$-correlation. Reactions with a positive ρ-value are accelerated (or the equilibrium constants of analogous equilibria are increased) by substituents with positive σ-constants. Since the sign of σ was defined so that substituents with a positive σ increase the acidity of benzoic acid, such substituents are generally described as attracting electrons away from the aromatic ring. It follows that reactions with a positive ρ-value are considered to involve a transition state (or reaction product) so that the difference in energy between this state and the reactants is decreased by a reduction in electron density at the reactive site of the substrate.
See also: Hammett equation, σ-constant, Taft equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1161

ρσ-equation (rho-sigma equation)

See: Hammett equation, ρ-value, σ-constant, Taft equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

R, *S*

The approved designations (devised by Cahn, Ingold and Prelog) of absolute configuration at four-coordinate (quadriligant) and six-coordinate (sexiligant) stereogenic centres.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

r, *s*

Stereodescriptor s of pseudo-asymmetric atoms

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

*R**, *S**

See: relative configuration

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

rabbit

A small container propelled pneumatically or hydraulically through a tube leading from the laboratory to a location in a nuclear reactor or other device where irradiation of a sample can take place.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1549

racemate

Also contains definitions of: *rac*, *RS*

Synonym: *SR*

An equimolar mixture of a pair of enantiomers. It does not exhibit optical activity. The chemical name or formula of a racemate is distinguished from those of the enantiomers by the prefix (±)- or *rac*- (or *racem*-) or by the symbols *RS* and *SR*.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

racemic

Pertaining to a racemate.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

racemic compound

A crystalline racemate in which the two enantiomers are present in equal amounts in a well defined arrangement within the lattice of a homogeneous crystalline addition compound.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

racemic conglomerate

Also contains definition of: spontaneous resolution

An equimolar mechanical mixture of crystals each one of which contains only one of the two enantiomers present in a racemate. The process of its formation on crystallization of a racemate is called spontaneous resolution, since pure or nearly pure enantiomers can often be obtained from the conglomerate by sorting.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

racemic mixture [obsolete]

The term is confusing since it has been used as a synonym for both racemate and racemic conglomerate. Usage strongly discouraged.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

racemization

The production of a racemate from a chiral starting material in which one enantiomer is present in excess.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

racemo structures

in polymers

See: meso structures *in polymers*

Source:
Purple Book, p. 37

rad

Non-SI unit of absorbed dose of radiation, $\mathrm{rad} = 0.01\ \mathrm{Gy}$.

Source:
Green Book, 2nd ed., p. 113
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 987

radial electrostatic field analyser

in mass spectrometry

An arrangement of two conducting sheets forming a capacitor and giving a radial electrostatic field which is used to deflect and focus ion beams of different energies. The capacitor may be cylindrical, spherical, or toroidal.

Source:
Orange Book, p. 201

radial elution (radial development) or circular elution (circular development)

in planar chromatography

A mode of operation in which the sample is spotted at a point source at or near the middle of the plane and is carried outward in a circle by the mobile phase, also applied at that place.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 829

radian

SI derived unit of plane angle, $\mathrm{rad} = 1$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 988

radiance, L

Radiant power, P, leaving or passing through a small transparent element of surface in a given direction from the source about the solid angle Ω, divided by the solid angle and by the orthogonally projected area of the element in a plane normal to the given beam direction, $\mathrm{d}S_{\perp} = \mathrm{d}S \cos\theta$

Notes:

1. Mathematical definition:

$$L = \frac{\mathrm{d}^2 P}{\mathrm{d}\Omega \, \mathrm{d}S_{\perp}} = \frac{\mathrm{d}^2 P}{\mathrm{d}\Omega \, \mathrm{d}S \cos\theta}$$

   for a divergent beam propagating in an elementary cone of the solid angle Ω containing the direction θ. SI unit is $\mathrm{W\ m^{-2}\ sr^{-1}}$.
2. For a parallel beam it is the radiant power, P, of all wavelengths leaving or passing through a small element of surface in a given direction from the source divided by the orthogonally projected area of the element in a plane normal to the given direction of the beam, θ. Mathematical definition in this case: $\mathrm{d}P / (\mathrm{d}S \cos\theta)$ If the radiant power is constant over the surface area considered, $P / (S \cos\theta)$. SI unit is $\mathrm{W\ m^{-2}}$.
3. Equivalent to $L = \int_{\lambda} L_{\lambda} \mathrm{d}\lambda$, where L_{λ} is the spectral radiance at wavelength λ.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 408

radiant energy, Q

The total energy emitted, transferred or received as radiation in a defined period of time ($Q = \int Q_\lambda \mathrm{d}\lambda$). It is the product of radiant power, P, and time, t: $Q = P\,t$ when the radiant power is constant over the time considered.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2268
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 988
Green Book, 2nd ed., p. 30
ISO 31-5: 1992 *(Quantities and Units - Part 5: Electricity and Magnetism.)*

radiant energy density, ρ, w

Radiant energy divided by the volume.

Source:
Green Book, 2nd ed., p. 30

radiant (energy) flux, P, Φ [obsolete]

This obsolete term is not recommended. In photochemistry, radiant power, P, is adopted. SI unit is W.
Note:
P is preferred, because in photochemistry, Φ is reserved for quantum yield.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 409

radiant exitance, M

Synonym: radiant emittance

Radiant power, P, emitted at all wavelengths by an element of surface containing the source point under consideration divided by the area of the source. SI unit is $\mathrm{W\ m^{-2}}$.
Notes:

1. Mathematical definition: $M = \mathrm{d}P / \mathrm{d}S$. If the radiant power P is constant over the surface area considered, $M = P / S$.
2. Equivalent to the integration of the radiant power leaving a source over the solid angle and over the whole wavelength range. Mathematical definition: $M = \int_\lambda M_\lambda \mathrm{d}\lambda$, where M_λ is the spectral radiant exitance at wavelength λ.
3. Same as spherical radiant exitance. Formerly called radiant emittance.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 409

radiant exposure, *H*

Radiant energy, Q, incident from all upward directions on an small sphere divided by the cross-sectional area of that sphere. SI unit is $\mathrm{J\ m^{-2}}$.
Notes:

1. Equivalent definition: Irradiance, E integrated over the time of irradiation.
2. Mathematical definition: $H = \mathrm{d}Q / \mathrm{d}S = \int_t E \mathrm{d}t$ If Q is constant over the area, $H = Q / S$. If E is constant over the time interval, $H = E\, t$.
3. This term refers to a beam not scattered or reflected by the target or its surroundings. For a beam incident from all directions fluence (H_o, F_o) is an equivalent term.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 409

radiant flux

See: radiant power

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 988

radiant intensity, *I*

Also contains definition of: intensity

Radiant power, P, at all wavelengths per solid angle, Ω. The radiant power emitted in a given direction by a source or an element of the source in a small cone containing the given direction divided by the solid angle of the cone. SI unit is $\mathrm{W\ sr^{-1}}$.
Notes:

1. Mathematical definition: $I = \mathrm{d}P / \mathrm{d}\Omega$. If the radiant power is constant over the solid angle considered, $I = P / \Omega$.
2. Equivalent to $I = \int_\lambda I_\lambda \mathrm{d}\lambda$, where I_λ is the spectral radiant intensity at wavelength λ.
3. It is not recommended to abbreviate this term to just intensity because it is confusing.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 410

radiant power, *P*

Power emitted, transferred or received as radiation. SI unit is $\mathrm{J\ s^{-1} = W}$.
Notes:

1. Mathematical definition: $P = \mathrm{d}Q / \mathrm{d}t$. If the radiant energy Q is constant over the time interval, $P = Q / t$.
2. In radiometry, flux (Φ) is used with the same units as P. The symbol Φ is reserved for quantum yield in photochemistry. Therefore, the use of flux (Φ) is not recommended.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 410

radiant quantities

Group of quantities characterizing electromagnetic radiation in terms of energy. The symbols of radiant quantities may be distinguished by adding a subscript e.

Source:
Green Book, 2nd ed., p. 30

radiation

A term embracing electromagnetic waves as well as fast moving particles. In radioanalytical chemistry the term usually refers to radiation emitted during a nuclear process (radioactive decay, nuclear reaction, nuclear fission, accelerators).

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523

radiation chemistry

The part of chemistry which deals with the chemical effects of ionizing radiation, as distinguished from photochemistry associated with visible and ultraviolet electromagnetic radiation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523
Orange Book, p. 236

radiation constants

Fundamental physical constants characterizing black body radiation. The first radiation constant is $c_1 = 2\,\pi\,h\,c_0^{\,2} = 3.741\ 7749(22) \times 10^{-16}\ \mathrm{W\ m^2}$, the second is

$c_2 = \frac{h\,c_0}{k} = 1.438\ 769(12) \times 10^{-2}$ m K, where h is the Planck constant c_0 the speed of light and k the Boltzmann constant.

Source:
CODATA Bull. 1986, *63*, 1

radiation continuum

in spectrochemistry

Continuous (in the wavelength, not time sense) radiation arising for example from non-quantized free-free transitions of electrons in the fields of the ions, free-bound transitions or radiative recombinations of electrons and ions, incandescent radiation emitted by hot solids (when the radiation distribution conforms to that described by Planck's law, it is considered black-body radiation) and unresolvable band spectra, i.e. where the spectral lines are wider than the spacings between them.

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1462

radiation counter

Radiation measuring assembly comprising a radiation detector in which individual ionizing events cause electrical pulses and the associated equipment for processing and counting the pulses. Often an expression is added indicating the type of radiation detector (e.g. scintillation, semiconductor).

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2516

radiation detector

Also contains definitions of: energy dispersive detector, nonselective detector, nonselective quantum counter, photochemical detector, photoelectric detector, selective detector, thermal detector

A device in which incident radiation produces a measurable effect. If this effect is a rise in temperature it is called a thermal detector. If it is a rise in pressure it is called a photoacoustic detector. In the case where an electrical signal is produced it is called a photoelectric detector. Photoelectric detectors can be classified as photo-emissive detectors and semiconductor detectors. Where the radiation produces a chemical reaction, it is termed a photochemical detector. A detector yielding an output signal that is independent of the wavelength of the radiation over a specific region is called a nonselective detector. Where it is wavelength specific it is a selective detector. A detector having a quantum efficiency independent of the wavelength is a nonselective quantum counter. Certain detectors are able to distinguish between different quantum energies. This property is described by the energy resolution ΔE and the energy resolving power $\frac{E}{\Delta E}$. These detectors are called energy dispersive detectors. In X-ray spectroscopy, the reciprocal $\frac{\Delta E}{E}$ is often used but this is discouraged.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1748
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518

radiation hazard

Hazard that exists in a region where there is a radiation field, other than what is considered to be normal background radiation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1549

radiation reaction

Chemical reaction that is induced by ionizing radiation with γ-ray, X-ray, electron, or other high-energy beams.
Notes:
1. Radiation reactions involving polymers often lead to chain scission and crosslinking.
2. A photochemical reaction is sometimes regarded as a type of radiation reaction.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 894

radiation spectrum

The components of radiation arranged in order of their wavelengths, frequencies or quantum energies. For particle radiation they are arranged in order of their kinetic energies.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1549

radiation trapping

Process by which the resonance radiation emitted in a lamp is absorbed and re-emitted many times in the plasma prior to striking the phosphor. This process is called radiation trapping or imprisonment.
Note:
Radiation trapping lengthens the effective lifetime of emission as viewed from outside the lamp. The control of this trapping is, therefore, an important design consideration for low-pressure lamps.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 410

radiationless deactivation

Also contains definition of: radiationless decay

Loss of electronic excitation energy without photon emission or chemical change. Often, ultrafast radiationless decays are mediated by conical intersections.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 410

radiationless transition

A transition between two states of a system without photon emission or absorption.
See also: radiative transition

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2269
Orange Book, p. 185

See also:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 234

radiative absorption

Also contains definitions of: transition probability for absorption *in spectrochemistry* , transition probability for stimulated emission *in spectrochemistry*

in spectrochemistry

A process by which a particle in the ground state or an excited state may undergo transition to a higher energy level by absorption of a photon. For a given particle in the lower state of probability per second of such a transition in a field with a continuous spectrum is proportional to the spectral radiant energy density of the absorption line. The proportionality constant is termed the transition probability for absorption. The transition probability for stimulated emission is defined in a similar way for the reverse radiative de-excitation process that is induced by the same radiation field.

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1463

radiative capture

Capture of a particle by a nucleus followed by immediate emission of gamma radiation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

radiative de-excitation

Also contains definition of: transition probability for spontaneous emission *in spectrochemistry*

in spectrochemistry

The change in the internal energy of a particle may be due to radiative processes, i.e. the emission or absorption of a photon. A particle in an excited state may undergo a transition to a lower energy level by emission of a photon. This is known as radiative de-excitation. If such a transition occurs spontaneously its probability per second for a given excited particle is termed the transition probability for spontaneous emission.

Source:
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1463

radiative energy transfer

Also contains definition of: trivial energy transfer

Transfer of excitation energy by radiative deactivation of a donor molecular entity and reabsorption of the emitted radiation by an acceptor molecular entity.
Notes:

1. Radiative transfer results in a decrease of the donor fluorescence intensity in the region of spectral overlap. Such a distortion of the fluorescence spectrum is called inner-filter effect.
2. Radiative energy transfer depends on the shape and size of the vessel utilized and on the configuration of the latter with respect to excitation and observation.
3. The fraction a of photons emitted by D and absorbed by A is given by

$$a = \frac{1}{\Phi_{\mathrm{D}}^{0}} \int_{\lambda} I_{\lambda}^{\mathrm{D}}(\lambda)\,[1 - 10^{-\varepsilon_{\mathrm{A}}(\lambda)\,c_{\mathrm{A}}\,l}]\mathrm{d}\lambda$$

where c_{A} is the molar concentration of acceptor, Φ_{D}^{0} is the fluorescence quantum yield in the absence of acceptor, l is the thickness of the sample, $I_{\lambda}^{\mathrm{D}}(\lambda)$ and $\varepsilon_{\mathrm{A}}(\lambda)$ are the spectral distribution of the spectral radiant intensity of the donor fluorescence and the molar decadic absorption coefficient of the acceptor, respectively, with the normalization condition $\Phi_{\mathrm{D}}^{0} = \int_{\lambda} I_{\lambda}^{\mathrm{D}}(\lambda)\mathrm{d}\lambda$.

For relatively low absorbance, a can be approximated by

$$a = \frac{2.3}{\Phi_{\mathrm{D}}^{0}}\, c_{\mathrm{A}}\, l \int_{\lambda} I_{\lambda}^{\mathrm{D}}(\lambda)\,\varepsilon_{\mathrm{A}}(\lambda)\mathrm{d}\lambda$$

where the integral represents the overlap between the donor fluorescence spectrum and the acceptor absorption spectrum.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 411

radiative lifetime, τ_0

Also contains definition of: natural lifetime

Lifetime of an excited molecular entity in the absence of radiationless transitions. The reciprocal of the first-order rate constant for the radiative step, or the reciprocal of the sum of these rate constants if there is more than one such step. The equivalent term, natural lifetime, is discouraged.
Notes:

1. Approximate expressions exist relating τ_0 to the oscillator strength of the emitting transition.
2. The subscript 0 is used in this definition, whereas the superscript 0 is used to indicate a non-quenched lifetime in the Stern-Volmer kinetic relationships.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 411

radiative transition

A transition between two states of a molecular entity, the energy difference being emitted or absorbed as photons. In principle, radiative and radiationless transitions can be distinguished in molecules. The first occur by absorption or emission of light quanta, and the latter is the result of the transformation of electronic excitation energy into vibrational/rotational energy.
See also: radiationless transition

Source:
Orange Book, p. 185
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2270
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 234

radical centre(s)

The atom (or group of atoms) in a polyatomic radical on which an unpaired electron is largely localized. Attachment of a monovalent atom to a radical centre gives a molecule for which it is possible to write a Lewis formula in which the normal stable valencies are assigned to all atoms.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1156

radical combination

See: colligation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1156

radical copolymerization

A copolymerization which is a radical polymerization.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2308

radical (free radical)

A molecular entity such as $^{\cdot}CH_3$, $^{\cdot}SnH_3$, $Cl^{\cdot}$ possessing an unpaired electron. (In these formulae the dot, symbolizing the unpaired electron, should be placed so as to indicate the atom of highest spin density, if this is possible.) Paramagnetic metal ions are not normally regarded as radicals. However, in the 'isolobal analogy' the similarity between certain paramagnetic metal ions and radicals becomes apparent. At least in the context of physical organic chemistry, it seems desirable to cease using the adjective 'free' in the general name of this type of chemical species and molecular entity, so that the term 'free radical' may in future be restricted to those radicals which do not form parts of radical pairs. Depending upon the core atom that possesses the unpaired electron, the radicals can be described as carbon-, oxygen-, nitrogen-, metal-centred radicals. If the unpaired electron occupies an orbital having considerable s or more or less pure p character, the respective radicals are termed σ- or π-radicals. In the past, the term 'radical' was used to designate a substituent group bound to a molecular entity, as opposed to 'free radical', which nowadays is simply called radical. The bound entities may be called groups or substituents, but should no longer be called radicals.
See also: biradical

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1155
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1362

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2209

radical ion

Also contains definitions of: anion radical, cation radical, radical anion, radical cation

A radical that carries an electric charge. A positively charged radical is called a 'radical cation' (e.g. the benzene radical cation $C_6H_6^{\cdot +}$); a negatively charged radical is called a 'radical anion' (e.g. the benzene radical anion $C_6H_6^{\cdot -}$ or the benzophenone radical anion $Ph_2C{-}O^{\cdot -}$). Commonly, but not necessarily, the odd electron and the charge are associated with the same atom. Unless the positions of unpaired spin and charge can be associated with specific atoms, superscript dot and charge designations should be placed in the order $^{\cdot +}$ or $^{\cdot -}$ suggested by the name 'radical ion'. (e.g. $C_3H_6^{\cdot +}$).
Note:
In the previous edition of this Compendium, it was recommended to place the charge designation directly above the centrally placed dot. However, this format is now discouraged because of the difficulty of extending it to ions bearing more than one charge, and/or more than one unpaired electron. In mass spectroscopic usage the symbol for the charge precedes the dot representing the unpaired electron.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1156
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1363

radical pair (geminate pair)

The term is used to identify two radicals in close proximity in solution, within a solvent cage. They may be formed simultaneously by some unimolecular process, e.g. peroxide decomposition, or they may have come together by diffusion. While the radicals are together, correlation of the unpaired electron spins of the two species cannot be ignored: this correlation is responsible for the CIDNP phenomenon. A radical pair is called geminate provided that each radical partner is a descendant of the same parental pair.
See also: geminate recombination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1156
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1363
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2270

radical photosubstitution

Also contains definition of: free-radical photosubstitution

Photo-induced substitution resulting from the reaction of radicals produced by photolysis of an appropriate reagent, such as, e.g., halogenated compounds.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 412

radical polymerization

A chain polymerization in which the kinetic-chain carriers are radicals.
Note:
Usually, the growing chain end bears an unpaired electron.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2308

radicofunctional name

See: functional class name

Source:
Blue Book (Guide), p. 14

radioactive

The property of a nuclide of undergoing spontaneous nuclear transformations with the emission of radiation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523

radioactive age

The time, estimated from measurement of the isotopic composition, during which the content of a radioactive species within an object has remained unchanged except for nuclear decay.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1549

radioactive contamination

A radioactive substance in a material or place where it is undesirable.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1549

radioactive cooling

Of a strongly radioactive material, the decrease of its activity by nuclear decay.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1538

radioactive dating

The determination of the radioactive age of an object from its content of radioactive substances and of their daughter products.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1539

radioactive decay

Nuclear decay in which particles or electromagnetic radiation are emitted or the nucleus undergoes spontaneous fission or electron capture.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2518

radioactive equilibrium

Among the members of a decay chain, the state which prevails when the ratios between the activities of successive members remain constant. (This is not an equilibrium in the strict sense since radioactive decay is an irreversible process).

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2519

radioactive fallout

The deposition on the ground of radioactive substances from nuclear explosions and other injections of radioactive material into the atmosphere.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

radioactive source

Any quantity of radioactive material which is intended for use as a source of ionizing radiation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

radioactive tracer

A tracer containing a radioactive label.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

radioactive tracer technique

in analysis

A technique for investigating recovery and loss of a microcomponent, in which a radioactively-labelled element or compound chemically identical with the microcomponent is added to the sample before preconcentration and its behaviour is followed by sensitive, rapid and selective radioactivity measurements.

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1200

radioactive waste

Unwanted radioactive materials obtained in the processing or handling of radioactive materials.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

radioactivity

The property of certain nuclides showing radioactive decay.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 988
Green Book, 2nd ed., p. 22

radiochemical activation analysis

A kind of activation analysis in which, after the irradiation, chemical or physical separation is applied.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515

radiochemical purification

Chemical separation applied to a radioactive preparation in order to improve the radiochemical purity.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

radiochemical purity

For a material, the fraction of the stated isotope present in the stated chemical form.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523

radiochemical separation

Separation by a chemical means of the radioactive isotopes of a specific element from a mixture of radionuclides.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

radiochemical yield

The yield of a radiochemical separation expressed as a fraction of the activity originally present.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

radiochemistry

That part of chemistry which deals with radioactive materials. It includes the production of radionuclides and their compounds by processing irradiated materials or naturally occurring radioactive materials, the application of chemical techniques to nuclear studies, and the application of radioactivity to the investigation of chemical, biochemical or biomedical problems.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radiochromatograph

A measuring assembly designed to measure the spatial or time distribution of the activity of a mixture of radioactive components after separation by a chromatographic method.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

radiocolloid

A colloid in which some atoms are radioactive.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

radioenzymatic assay

An assay of the catalytic activity of an enzyme based on the use of a radioactive substrate.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radiograph

A visual representation of an object produced by placing the object between a source of ionizing radiation and a photographic plate or film.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radiogravimetric analysis

A kind of quantitative analysis in which the activity of a precipitate is used as a measure of its mass.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radioimmunoassay

An assay based on the reversible and non-covalent binding of an antigen (hapten) by a specific antibody employing radioactivity labelled antigen (hapten) to measure the fraction of the antigen (hapten) bound to a substoichiometric amount of antibody.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radioiodination

The process of incorporating the radionuclides of iodine (usually ^{125}I, ^{131}I or ^{123}I) into, or of covalently linking a radioiodinated substance to, a substance.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radioisotope

A radioactive isotope of a specified element.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radioisotope dilution analysis

A kind of isotope dilution analysis making use of a radionuclide.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radioisotope induced X-ray emission analysis

A kind of analysis based on the measurement of the energies and intensities of characteristic X-radiation emitted by a test portion during irradiation with a radioactive source.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

radioluminescence

Luminescence arising from excitation by high-energy particles or radiation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2270

radiolysis

The cleavage of one or several bonds resulting from exposure to high-energy radiation. The term is also often used loosely to specify the method of irradiation ('pulse radiolysis') used in any radiochemical reaction, not necessarily one involving bond cleavage.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1156
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radiometric analysis

A kind of quantitative analysis in which measurement of the activity is an essential step.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radiometric titration

A titration in which a radioactive indicator is used to monitor the end-point of the titration.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radiometry

The measurement of quantities associated with radiant energy. The quantities may also describe the variation of the energy with respect to other variables such as wavelength, time, position, direction (solid angle), area normal to the light or projected area of emitting or receiving surfaces. If the light is monochromatic, it is sometimes convenient to replace the radiant energy by the corresponding number of photons (or quanta) which is obtained by dividing the energy by $\frac{h\,c}{\lambda}$ where h is the Planck constant, c the velocity of light and λ the wavelength of the light.
See: intensity, radiance, irradiance

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2209

radionuclide

A nuclide that is radioactive.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radionuclidic purity

For a material, that fraction of the total activity which is present in the form of the stated radionuclide, including daughter products.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2523

radioreceptor assay

An assay employing a radioactively labelled receptor protein as a tracer.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radiorelease analysis

A kind of quantitative analysis based on the release of radioactivity from the reagent by reaction with the analyte.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

radiosonde

A miniature radio transmitter with instruments in a package that is carried aloft (e.g. by an unmanned balloon) for broadcasting every few seconds by means of precise tone signals or other suitable method, the humidity, temperature, pressure or other parameter.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2209

radius of gyration, s

A parameter characterizing the size of a particle of any shape. For a rigid particle consisting of mass elements of mass m_i, each located at a distance r_i from the centre of mass, the radius of gyration, s, is defined as the square root of the mass-average of r_i^2 for all the mass elements, i.e.

$$s = \sqrt{\frac{\sum_i m_i r_i^2}{\sum_i m_i}}$$

For a non-rigid particle, an average over all conformations is considered, i.e.

$$\sqrt{< s^2 >} = \frac{\sqrt{< \sum_i m_i r_i^2 >}}{\sqrt{\sum_i m_i}}$$

The subscript zero is used to indicate unperturbed dimensions, as in $< s^2 >_0^{1/2}$.

Source:
Purple Book, p. 48

raffinate

The phase remaining after extraction of some specified solute(s). When necessary it should be further specified, e.g. scrub raffinate. The original meaning of raffinate as a 'refined product' has become extended and changed by common usage. The term should normally be applied only to waste streams but the latter may form the feed to a further extraction process for another solute.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2388

rain out

in atmospheric chemistry

The mechanism by which small particles in the clouds are removed by the formation of raindrops; this is a different mechanism from wash out which is a process which occurs below cloud level. Both the terms rain out and wash out have not always been used in accordance with these definitions. For clarity they should be replaced by the terms, in-cloud scavenging and below-cloud scavenging, respectively.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2209

random coil

Synonym: statistical coil *in polymers*

in polymers

The complete set of spatial arrangements of a chain molecule with a large number of segments that randomly change mutual orientation with time, under conditions in which it is free from external constraints that would affect its conformation. If the solution of the chain molecules is not in a theta state, the segments change mutual orientation only approximately randomly. Synonymous with statistical coil.

Source:
Purple Book, p. 50

random coincidence

in nuclear chemistry

A coincidence of events occurring in not physically connected nuclei.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

random copolymer

A copolymer consisting of macromolecules in which the probability of finding a given monomeric unit at any given site in the chain is independent of the nature of the adjacent units.
Note:
In a random copolymer, the sequence distribution of monomeric units follows Bernoullian statistics.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2301

random copolymerization

A copolymerization in which a random copolymer is formed.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2307

random error

Result of a measurement minus the mean that would result from an infinite number of measurements of the same measurand carried out under repeatability conditions.
See also: measurement result

Source:
VIM

random sample

The sample so selected that any portion of the population has an equal (or known) chance of being chosen. Haphazard or arbitrary choice of units is generally insufficient to guarantee randomness.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1202

range [obsolete]

in analysis

The difference between the highest and lowest members of a series. This term is not recommended.

Source:
Orange Book, p. 5

See also:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 599

range of measurement

of an analyser

The range of concentration between the measurement threshold and the maximum usable indication.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

rate

Derived quantity in which time is a denominator quantity. Rate of x is $\frac{\mathrm{d}x}{\mathrm{d}t}$.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 988

rate coefficient

See: order of reaction, kinetic equivalence

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1157

rate law (empirical differential rate equation)

An expression for the rate of reaction of a particular reaction in terms of concentrations of chemical species and constant parameters (normally rate coefficients and partial orders of reaction) only. For examples of rate laws see equations (1)-(3) under kinetic equivalence, and (1) under steady state.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1157

rate of change of a quantity

The time derivative $\frac{\mathrm{d}Q}{\mathrm{d}t}$ of the value of the quantity. The differential quotient may also be called derivative (or instantaneous) rate of change. Examples are: rate of change of mass, $\frac{\mathrm{d}m}{\mathrm{d}t}$; rate of change of amount of substance, $\frac{\mathrm{d}n}{\mathrm{d}t}$.

Source:
PAC, 1992, *64*, 1569 *(Quantities and units for metabolic processes as a function of time (IUPAC Recommendations 1992))* on page 1572

rate of change ratio

The quotient of two rates where the quantities are of the same kind in the same system for different components:

$$\frac{\mathrm{d}Q_1 / \mathrm{d}t}{\mathrm{d}Q_2 / \mathrm{d}t}$$

For finite time intervals, mean rate of change ratio is:

$$\frac{\Delta Q_1 / \Delta t}{\Delta Q_2 / \Delta t} = \frac{\Delta Q_1}{\Delta Q_2}\,\Delta t$$

Rate of change ratio has the dimension one. The denominator is often called the reference quantity. Examples are: mass rate ratio, $\frac{\mathrm{d}m_1 / \mathrm{d}t}{\mathrm{d}m_2 / \mathrm{d}t}$; amount of substance rate ratio, $\frac{\mathrm{d}n_1 / \mathrm{d}t}{\mathrm{d}n_2 / \mathrm{d}t}$.

Source:
PAC, 1992, *64*, 1569 *(Quantities and units for metabolic processes as a function of time (IUPAC Recommendations 1992))* on page 1572

rate of consumption, $v_{n,\mathrm{B}}$ or $v_{c,\mathrm{B}}$

The rate of consumption of a specified reactant may be defined in two ways:

1. As the negative of the time derivative of the amount of reactant; thus for a reactant B, present at any time in amount n_B, the rate of its consumption may be defined as:

   $$v(n_\mathrm{B}) = -\frac{\mathrm{d}n_\mathrm{B}}{\mathrm{d}t}$$

   This definition is particularly appropriate for open systems. Here and elsewhere, when a rate is defined in terms of a time derivative, it must be understood that the definition relates to the process occurring in isolation. In a flow system there may be no actual changes with time, and the time derivative must be inferred. Such an inference is also required for a reaction occurring by a composite mechanism.

2. For kinetics in closed systems it is more usual to define a rate of consumption per unit volume; thus for a reactant B the rate of consumption, $v(c_B)$ is given by:

$$v(c_B) = -\frac{1}{V}\frac{dn_B}{dt}$$

When the volume V is constant this reduces to:

$$v(c_B) = -\frac{d[B]}{dt}$$

When the volume is not constant the relationship $n_B = [B]\ V$ may be differentiated to give:

$$dc_B = V\,d[B] + [B]\ dV$$

and therefore:

$$v(c_B) = -\frac{d[B]}{dt} - \frac{[B]}{V}\frac{dV}{dt}$$

In contrast to the rate of conversion and the rate of reaction, the rate of consumption of a reactant may be specified even for a reaction of time-dependent stoichiometry or of unknown stoichiometry. The rate of consumption of a reactant is often called its rate of disappearance. However, the former expression is to be preferred since the word disappearance is not appropriately translatable into certain languages. When English is used the word disappearance might be reserved for cases where the reactant is almost completely removed.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 179

rate of conversion, $\dot{\xi}$

The rate of conversion for a reaction occurring in a closed system is defined as the time derivative of the extent of reaction:

$$\dot{\xi} = \frac{d\xi}{dt}$$

In view of the definition of extent of reaction it follows that with reference to any species in a reaction showing time-independent stoichiometry

$$\dot{\xi} = \frac{d\xi}{dt} = \frac{1}{\nu_i}\frac{dn_i}{dt}$$

where n_i is the amount of the species at any time and ν_i is its stoichiometric coefficient.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 180

PAC, 1992, *64*, 1569 *(Quantities and units for metabolic processes as a function of time (IUPAC Recommendations 1992))* on page 1573
Green Book, 2nd ed., p. 55
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 989

rate of disappearance

See: rate of reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1157

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 181

rate of fluid consumption, q_V

in flame emission and absorption spectrometry

The volume of fluid consumed by the nebulizer divided by time (in $\mu L\ s^{-1}$). Volume rate has also been called volume flow, flux, aspiration rate, aspiration flow or aspiration flux. The fluid consumed is either aspirated or injected. The volume rate of fluid consumption by nebulizers is usually between 10 and 100 $\mu L\ s^{-1}$.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1739

rate of formation, $v_{n,\mathrm{y}}$ or $v_{c,\mathrm{y}}$

Like the rate of consumption, the rate of formation of a specified product may be defined in two ways:

1. As the time derivative of the amount of a product. Thus for a product Y, present at any time in amount n_Y. the rate of its formation may be given by:

   $$v(n_\mathrm{Y}) = \frac{\mathrm{d}n_\mathrm{Y}}{\mathrm{d}t}$$

   This definition is particularly appropriate for open systems.
2. For kinetics in closed systems it is more usual to define a rate of formation per unit volume, denoted $v(c_\mathrm{Y})$:

   $$v(c_\mathrm{Y}) = \frac{1}{V}\frac{\mathrm{d}n_\mathrm{Y}}{\mathrm{d}t}$$

   When the volume is constant this reduces to:

$$v(c_{\mathrm{Y}}) = \frac{1}{V}\frac{\mathrm{d}n_{\mathrm{Y}}}{\mathrm{d}t} = \frac{\mathrm{d}[\,\mathrm{Y}\,]}{\mathrm{d}t}$$

When the volume is not constant the relationship $n_{\mathrm{Y}} = [\,\mathrm{Y}\,]\,V$ may be differentiated to give:

$$\mathrm{d}n_{\mathrm{Y}} = V\,\mathrm{d}[\,\mathrm{Y}\,] + [\,\mathrm{Y}\,]\,\mathrm{d}V$$

and the rate of formation becomes:

$$v(c_{\mathrm{Y}}) = \frac{\mathrm{d}[\,\mathrm{Y}\,]}{\mathrm{d}t} + \frac{[\,\mathrm{Y}\,]}{V}\frac{\mathrm{d}V}{\mathrm{d}t}$$

A rate of formation may be specified even for a reaction of time dependent stoichiometry or of unknown stoichiometry.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 181

rate of liquid consumption

in flame spectroscopy

The volume of liquid sample that is consumed by the nebulizing system per unit of time.

Source:
Orange Book, p. 166

rate of migration, v

in electrophoresis

The distance of migration divided by time, sometimes called velocity of migration. The symbol v is also used for velocity.

Source:
PAC, 1994, *66*, 891 *(Quantities and units for electrophoresis in the clinical laboratory (IUPAC Recommendations 1994))* on page 895

rate of nucleation

The number of nuclei formed in unit time per unit volume of the liquid phase.

Source:
Orange Book, p. 84

See also:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

rate of reaction, v

Also contains definition of: rate of appearance

For the general chemical reaction :

$$aA + bB \rightarrow pP + qQ + ...$$

occurring under constant-volume conditions, without an appreciable build-up of reaction intermediates, the rate of reaction v is defined as:

$$v = -\frac{1}{a}\frac{d[A]}{dt} = -\frac{1}{b}\frac{d[B]}{dt} = \frac{1}{p}\frac{d[P]}{dt} = \frac{1}{q}\frac{d[Q]}{dt}$$

where symbols placed inside square brackets denote amount (or amount of substance) concentrations (conventionally expressed in units of $\mathrm{mol\ dm^{-3}}$). The symbols R and r are also commonly used in place of v. It is recommended that the unit of time should always be the second. In such a case the rate of reaction differs from the rate of increase of concentration of a product P by a constant factor (the reciprocal of its coefficient in the stoichiometric equation, p) and from the rate of decrease of concentration of the reactant A by α^{-1}. The quantity:

$$\dot{\xi} = \frac{d\xi}{dt}$$

defined by the equation:

$$\dot{\xi} = -\frac{1}{a}\frac{dn_A}{dt} = -\frac{1}{b}\frac{dn_B}{dt} = \frac{1}{p}\frac{dn_P}{dt} = \frac{1}{q}\frac{dn_Q}{dt}$$

(where n_A designates the amount of substance A, conventionally expressed in units of mole) may be called the 'rate of conversion' and is appropriate when the use of concentrations is inconvenient, e.g. under conditions of varying volume. In a system of constant volume, the rate of reaction is equal to the rate of conversion per unit volume throughout the reaction. For a stepwise reaction this definition of 'rate of reaction' (and 'extent of reaction', ξ) will apply only if there is no accumulation of intermediate or formation of side products. It is therefore recommended that the term 'rate of reaction' be used only in cases where it is experimentally established that these conditions apply. More generally, it is recommended that, instead, the terms 'rate of disappearance' or 'rate of consumption' of A (i.e. $-\frac{d[A]}{dt}$, the rate of decrease of concentration of A) or 'rate of appearance' of P (i.e. $\frac{d[P]}{dt}$, the rate of increase of concentration of product P) be used, depending on the concentration change of the particular chemical species that is actually observed. In some cases reference to the chemical flux observed may be more appropriate. The symbol v (without lettered subscript) should be used only for rate of reaction; v with a lettered subscript (e.g. v_A) refers to a rate of appearance or rate of disappearance (e.g. of the chemical species A).

See also: chemical relaxation, lifetime, order of reaction

Source:

PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1157

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 181

rate-controlling step

A rate-controlling (rate-determining or rate-limiting) step in a reaction occurring by a composite reaction sequence is an elementary reaction the rate constant for which exerts a strong effect — stronger than that of any other rate constant — on the overall rate. It is recommended that the expressions rate-controlling, rate-determining and rate-limiting be regarded as synonymous, but some special meanings sometimes given to the last two expressions are considered under a separate heading. A rate-controlling step can be formally defined on the basis of a control function (or control factor) CF, identified for an elementary reaction having a rate constant k_i by:

$$\mathrm{CF} = \frac{\partial(\ln v)}{\partial \ln k_i}$$

where v is the overall rate of reaction. In performing the partial differentiation all equilibrium constants K_j and all rate constants except k_i are held constant. The elementary reaction having the largest control factor exerts the strongest influence on the rate v, and a step having a CF much larger than any other step may be said to be rate-controlling. A rate-controlling step defined in the way recommended here has the advantage that it is directly related to the interpretation of kinetic isotope effects. As formulated this implies that all rate constants are of the same dimensionality. Consider however the reaction of A and B to give an intermediate C, which then reacts further with D to give products:

$$\mathrm{A} + \mathrm{B} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{C} \qquad (1)$$

$$\mathrm{C} + \mathrm{D} \xrightarrow{k_2} \text{Products} \qquad (2)$$

Assuming that C reaches a steady state, then the observed rate is given by:

$$v = \frac{k_1 k_2 [\mathrm{A}][\mathrm{B}][\mathrm{D}]}{k_{-1} + k_2 [\mathrm{D}]}$$

Considering $k_2[\mathrm{D}]$ a pseudo-first order rate constant, then $k_2[\mathrm{D}] \gg k_{-1}$, and the observed rate $v = k_1[\mathrm{A}][\mathrm{B}]$ and $k_{\mathrm{obs}} = k_1$. Step (1) is said to be the rate-controlling step. If $k_2[\mathrm{D}] \ll k_{-1}$, then the observed rate:

$$v = \frac{k_1 k_2}{k_{-1}} [\mathrm{A}][\mathrm{B}][\mathrm{D}] = K k_2 [\mathrm{A}][\mathrm{B}][\mathrm{D}]$$

where K is the equilibrium constant for the pre-equilibrium (1) and is equal to $\frac{k_1}{k_{-1}}$, and $k_{\text{obs}} = K\,k_2$. Step (2) is said to be the rate-controlling step.
See also: Gibbs energy diagram, microscopic diffusion control, mixing control, rate-determining step

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1156

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 182

rate-determining step (rate-limiting step)

These terms are best regarded as synonymous with rate-controlling step. However, other meanings that have been given to them should be mentioned, as it is necessary to be aware of them in order to avoid confusion. Sometimes the term rate-determining is used as a special case of rate-controlling, being assigned only to an initial slow step which is followed by rapid steps. Such a step imposes an upper limit on the rate, and has also been called rate-limiting. In view of the considerable danger of confusion when special meanings are applied to rate-determining and rate-limiting, it is recommended that they be regarded as synonymous, with the meaning explained under the entry rate-controlling step.
See: Michaelis–Menten kinetics

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1157

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 183

ratemeter

in radiochemistry

An electronic sub-assembly which gives a continuous indication proportional to the average counting rate over a predetermined time interval (time constant).

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1550

ratio

Quotient of quantities of the same kind for different components within the same system.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 989

PAC, 1985, *57*, 1299 *(Review of plasma deposition applications: preparation of optical waveguides)* on page 1309

raw coke

The term raw coke is equivalent to green coke although it is now used less frequently.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 503

Rayleigh ratio

The quantity used to characterize the scattered intensity at the scattering angle θ, defined as $R(\theta) = \frac{i_\theta r^2}{I f V}$, where I is the intensity of the incident radiation, i_θ is the total intensity of scattered radiation observed at an angle θ and a distance r from the point of scattering and V is the scattering volume. The factor f takes account of polarization phenomena. It depends on the type of radiation employed.

1. For light scattering, dependent on the polarization of the incident beam, $f = 1$ for vertically polarized light, $f = \cos^2 \theta$ for horizontally polarized light and $f = \frac{1 + \cos^2 \theta}{2}$ for unpolarized light.
2. For small-angle neutron scattering, $f = 1$.
3. For small-angle X-ray scattering, $f \approx 1$, if $\theta < \text{ca. } 5\ ^\circ$.

Notes:

1. The dimension of $R(\theta)$ is $(\text{length})^{-1}$.
2. In small-angle neutron scattering the term cross-section is often used instead of $R(\theta)$; the two quantities are identical.
3. An alternative recommended symbol is R_θ.

Source:
Purple Book, p. 65

Rayleigh scattering

The scattering of light by particles and molecules which are much smaller than the wavelength of the light. In the ideal case, the process is one of pure dipole and induced dipole interactions with the electric field of the light wave. The scattering cross section for light of wavelength λ is proportional to λ^{-4}.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2209

rayon-based carbon fibres

Carbon fibres made from rayon (cellulose) precursor fibres.
Note:
Rayon-based carbon fibres have a more isotropic structure than similarly heat-treated polyacrylonitrile (PAN)- or mesophase pitch (MPP)-based carbon fibres. Their Young's modulus values are therefore drastically lower ($100\ \mathrm{GPa}$; tensile strength $100\ \mathrm{MPa}$). Rayon-based carbon fibres can be transformed into anisotropic carbon fibres with high strength and Young's modulus values by hot-stretching treatment at temperatures of approximately $2800\ \mathrm{K}$.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 503

Re, *Si*

A stereoheterotopic face of a trigonal atom is designated *Re* if the ligands of the trigonal atom appear in a clockwise sense in order of CIP priority when viewed from that side of the face. The opposite arrangement is termed *Si*.
See also: enantiotopic, and illustrated under prochirality.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

re-extraction **[obsolete]**

Since the prefix 're' can signify 'back' as well as 'again' this term is ambiguous and should be avoided, except where the process of *extraction* (e.g. from aqueous solution to an organic phase) in a single direction is repeated (following stripping). It should not be used as a synonym for stripping or back-extraction.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2379

reactance, X

Imaginary part of the impedance.

Source:
Green Book, 2nd ed., p. 15

reactant

A substance that is consumed in the course of a chemical reaction. It is sometimes known, especially in the older literature, as a reagent, but this term is better used in a more specialized sense as a test substance that is added to a system in order to bring about a reaction or to see whether a reaction occurs (e.g. an analytical reagent).

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 183

reacting bond rules

1. For an internal motion of a molecular entity corresponding to progress over a transition state (energy maximum), any change that makes the motion more difficult will lead to a new molecular geometry at the energy maximum, in which the motion has proceeded further. Changes that make the motion less difficult will have the opposite effect. (This rule corresponds to the Hammond principle).
2. For an internal motion of a molecular entity that corresponds to a vibration, any change that tends to modify the equilibrium point of the vibration in a particular direction will actually shift the equilibrium in that direction.
3. Effects on reacting bonds (bonds made or broken in the reaction) are the most significant. The bonds nearest the site of structural change are those most strongly affected.

See also: More O'Ferrall–Jencks diagram

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1158

reaction

See: chemical reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1158

reaction barrier

The energy barrier to chemical reaction. In vibrationally adiabatic transition-state theory its height is the zero-point energy of the activated complex minus that of the reactants.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 183

reaction chromatography

A technique in which the identities of the sample components are intentionally changed between sample introduction and detection. The reaction can take place upstream of the column when the chemical identity of the individual components passing through the column differs from that of the original sample, or between the column and the detector when the original sample components are separated in the column but their identity is changed prior to entering the detection device.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 827

reaction coordinate

A geometric parameter that changes during the conversion of one (or more) reactant molecular entities into one (or more) product molecular entities and whose value can be taken for a measure of the progress of an elementary reaction (for example, a bond length or bond angle or a combination of bond lengths and/or bond angles; it is sometimes approximated by a non-geometric parameter, such as the bond order of some specified bond). In the formalism of ' transition-state theory ', the reaction coordinate is that coordinate in a set of curvilinear coordinates obtained from the conventional ones for the reactants which, for each reaction step, leads smoothly from the configuration of the reactants through that of the transition state to the configuration of the products. The reaction coordinate is typically chosen to follow the path along the gradient (path of shallowest ascent/deepest descent) of potential energy from reactants to products. The term has also been used interchangeably with the term transition coordinate, applicable to the coordinate in the immediate vicinity of the potential energy maximum. Being more specific, the name transition coordinate is to be preferred in that context.
See also: potential-energy profile, potential-energy reaction surface, minimum-energy reaction path

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1158
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 183

reaction cross-section, σ_r

A quantity used in collision theories of reactions in order to interpret calculated or experimental rates. In some collision theories the reaction cross-section is considered to be related to b_max, the maximum value of the impact parameter that allows reaction to occur, by:

$$\sigma_\mathrm{r} = P_\mathrm{r}\, \pi\, b_\mathrm{max}{}^2$$

where P_r is the reaction probability.
See: collision cross-section

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 183

reaction dynamics

A branch of chemical kinetics that is concerned with the intermolecular and intramolecular motions that occur in the elementary act of chemical change, and with the details of the relationships between the quantum states of the reactant molecules and those of the product molecules. It is also known as molecular dynamics.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 184

reaction injection moulding

Acronym: RIM

Reactive polymer processing that produces polymer monoliths by low-pressure injection and mixing of low-viscosity precursors into moulds.
Note:
Reaction injection moulding commonly uses two-component precursors that produce polymer networks after mixing.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1824

reaction intermediate

See: intermediate

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1126

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 170

reaction path

1. A synonym for mechanism.
2. A trajectory on the potential-energy surface.
3. A sequence of synthetic steps.

See also: minimum-energy reaction path

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1159

reaction path degeneracy

Also contains definition of: statistical factor

A factor that is introduced into rate theory to take account of the fact that the process may be able to occur in different but equivalent ways. Thus the process:

$$\mathrm{Cl} + \mathrm{H_2} \longrightarrow \mathrm{HCl} + \mathrm{H}$$

has a reaction path degeneracy of 2 since the chlorine atom can abstract either of the two hydrogen atoms in the hydrogen molecule. The reaction path degeneracy has also been referred to as the statistical factor for the reaction.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 184

reaction probability, P_r

The probability that a reaction occurs when two particles undergo a collision. If N_c is the number of collisions occurring in unit time, and N_r the number of reactions occurring in unit time: $P_\mathrm{r} = \frac{N_\mathrm{r}}{N_\mathrm{c}}$.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 184

reaction stage

A set of one or more (possibly experimentally inseparable) reaction steps leading to and/or from a detectable or presumed reaction intermediate.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1159

reaction step

An elementary reaction, constituting one of the stages of a stepwise reaction in which a reaction intermediate (or, for the first step, the reactants) is converted into the next reaction intermediate (or, for the last step, the products) in the sequence of intermediates between reactants and products.
See also: rate-limiting step, reaction stage

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1159

reaction time

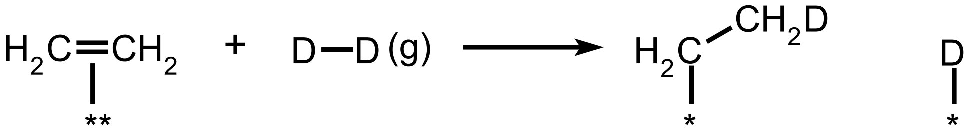
The period of time that elapses between the start of the reaction and the attainment of a given extent of a reaction.

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2297

reactive adsorption

Also contains definition of: reactive desorption

Reactive adsorption (and its reverse, reactive desorption) resembles dissociative adsorption (and its reverse, associative desorption) but one fragment adds to an adsorbate rather than to a surface site.



Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 84

reactive blending

Mixing process that is accompanied by the chemical reaction(s) of components of a polymer mixture.
Notes:

1. Examples of reactive blending are: (a) blending accompanied by the formation of a polymer-polymer complex, (b) the formation of block or graft copolymers by a combination of radicals formed by the mechano-chemical scission of polymers during blending.
2. Reactive blending may also be carried out as reactive extrusion or reaction injection molding (RIM).

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 894

reactive complex

A species of very short life that occurs as an intermediate in a chemical reaction. An activated complex (or transition state) is a special case.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 184

reactive polymer

Polymer having reactive functional groups that can undergo chemical transformation under the conditions required for a given reaction or application.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 897

reactive polymer processing

Process whereby a polymeric monolith is produced through an *in-situ* polymerization or polymer modification reaction.
Notes:

1. The polymerization or modification reaction and the transformation of the resulting polymer into a shaped product is accomplished in the same processing equipment.
2. This type of processing is commonly accomplished by extrusion or injection moulding.
3. Reaction injection moulding and reinforced reaction injection moulding are types of reactive polymer processing.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1825

reactive (reactivity)

As applied to a chemical species, the term expresses a kinetic property. A species is said to be more reactive or to have a higher reactivity in some given context than some other (reference) species if it has a larger rate constant for a specified elementary reaction. The term has meaning only by reference to some explicitly stated or implicitly assumed set of conditions. It is not to be used for reactions or reaction patterns of compounds in general. The term is also more loosely used as a phenomenological description not restricted to elementary reactions. When applied in this sense the property under consideration may reflect not only rate, but also equilibrium, constants.
See also: stable, unreactive, unstable

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1159

reactive scattering

If in a molecular-beam experiment a chemical reaction occurs there is said to be reactive scattering.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 184

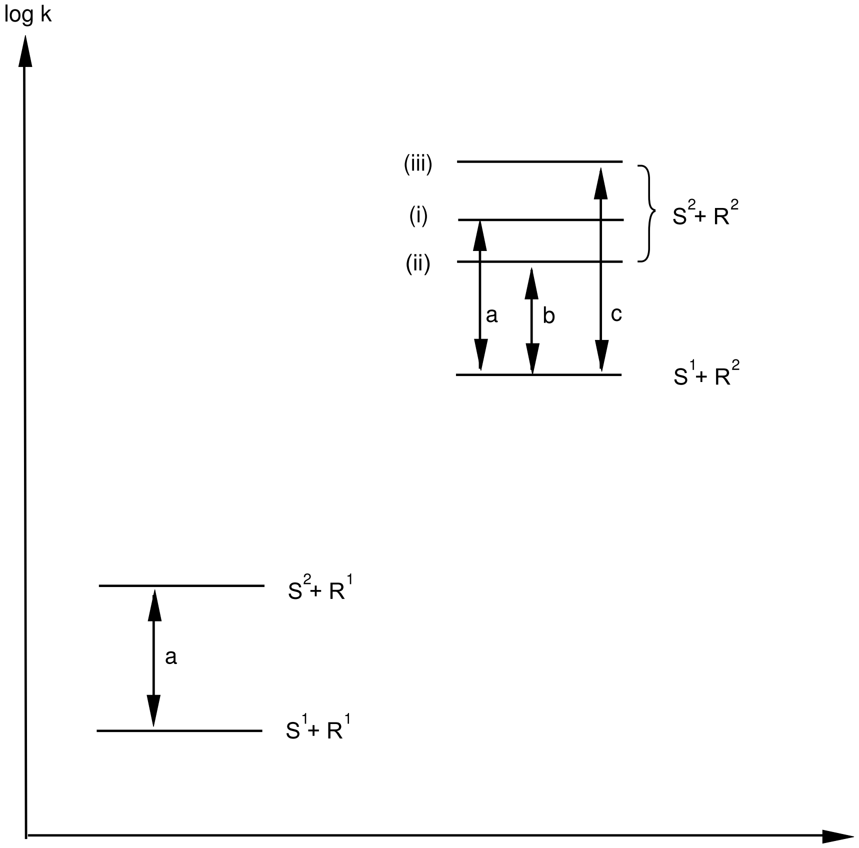
reactivity index

Any numerical index derived from quantum mechanical model calculations that permits the prediction of relative reactivities of different molecular sites. Many indices are in use, based on a variety of theories and relating to various types of reaction. The more successful applications have been to the substitution reactions of conjugated systems where relative reactivities are determined largely by changes of π-electron energy.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1159

reactivity–selectivity principle (RSP)

This idea may be expressed loosely as: the more reactive a reagent is, the less selective it is. Consider two substrates S^1 and S^2 undergoing the same type of reaction with two reagents R^1 and R^2, S^2 being more reactive than S^1, and R^2 more reactive than R^1 in the given type of reaction. The relative reactivities (in log units, ***See:*** selectivity) for the four possible reactions may notionally be represented as shown in the diagram.



With the positions of ($S^1 + R^1$), ($S^2 + R^1$) and ($S^1 + R^2$) fixed, there are three types of positions for ($S^2 + R^2$). In position (i) the selectivity of R^2 for the two substrates, measured by a, is the same as the selectivity of R^1 for the two substrates, also a. In position (ii) the selectivity of R^2 for the two substrates, measured by b, is less than the selectivity of R^1 for the two substrates, i.e. $b < a$. It is this situation which is in accord with the RSP. In position (iii) the selectivity of R^2 for the two substrates, measured by c, is greater than the selectivity of R^1 for the two substrates, i.e. $c > a$. This situation may be described as anti-RSP. There are many examples in which the RSP is followed, but there are also many examples corresponding to situations (i) and (iii). The RSP is in accord with intuitive feeling and certainly holds in the limiting case when reactivity is controlled by diffusion. However, the validity of the RSP is a matter of great controversy.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1159

readability

of a balance

The smallest fraction of a division to which the index scale can be read with ease either by estimation or by the use of a vernier. It should normally be expressed in divisions of the pointer scale.

Source:
Orange Book, p. 36

reading

Datum provided by an instrument.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1662

reagent

See: reactant

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 183

real (electrified) interphase

See: electrified interphase

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

real potential of a species in a phase

Defined for species B in phase β as

$$\alpha_{\mathrm{B}}^{\beta} = \mu_{\mathrm{B}}^{\beta} - z_{\mathrm{B}}\, F\, \psi^{\beta}$$

where μ_{B}^{β} is the electrochemical potential of species B in phase β, z_{B} is the charge number of species B, F is the Faraday constant, and ψ^{β} is the outer electric potential of phase β. Since ψ^{β} is zero when the charge on the phase β is zero, the real potential may be regarded as the value of the electrochemical potential of the uncharged phase.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 506

real surface (interface) area

See: extent of an interface (surface)

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

rearrangement

See: degenerate rearrangement, molecular rearrangement, sigmatropic rearrangement

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1160

rearrangement ion

in mass spectrometry

An electrically charged species, involving a molecular or parent ion, in which atoms or groups of atoms have transferred from one portion of a molecule or molecular moiety to another during the ionization fragmentation processes.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550
Orange Book, p. 205

rearrangement stage

The elementary reaction or reaction stage (of a molecular rearrangement) in which there is both making and breaking of bonds between atoms common to a reactant and a reaction product or a reaction intermediate. If the rearrangement stage consists of a single elementary reaction, this is a 'rearrangement step'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1160

rebound reaction

If in a chemical process, occurring in a molecular beam, the reaction products are scattered backwards with respect to the moving centre of mass of the system, the reaction is called a rebound reaction.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 185

receptor

Molecular structure in or on a cell that specifically recognizes and binds to a compound and acts as a physiological signal transducer, or mediator of, an effect.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1067
This definition replaces an earlier definition of receptor.

receptor

in drug design

A receptor is a protein or a protein complex in or on a cell that specifically recognizes and binds to a compound acting as a molecular messenger (neurotransmitter, hormone, lymphokine, lectin, drug, *etc*). In a broader sense, the term receptor is often used as a synonym for any specific (as opposed to non-specific such as binding to plasma proteins) drug binding site, also including nucleic acids such as DNA.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1149

recognition site

1. A nucleotide sequence to which a protein binds specifically.
2. An amino acid sequence in an antibody molecule to which the specific antigen binds specifically.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 164

recoil

in radioanalytical chemistry

The motion acquired by a particle through a collision with, or the emission of, another particle or electromagnetic radiation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

recoil labelling

Labelling by a chemical reaction initiated by recoil.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

recoil-free fraction

in Mössbauer spectrometry

The fraction of all Mössbauer gamma rays of the transition which are emitted or absorbed without significant recoil energy loss.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 214

recombinant DNA technology

See: gene manipulation

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 164

reconstructive transition

A transition which involves a major reorganization of the crystal structure and a change of local topology, during which primary bonds are broken and reformed so that there is no immediate relationship between the crystal structures of the parent and product phases. Examples: The transition of Mg_2SiO_4 (olivine) to Mg_2SiO_4 (spinel); the transition of diamond to graphite.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 589

recovery

1. In toxicology, the process leading to partial or complete restoration of a cell, tissue, organ or organism following its damage from exposure to a harmful substance or agent.
2. Term used in analytical and preparative chemistry to denote the fraction of the total quantity of a substance recoverable following a chemical procedure.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2089

recovery factor [obsolete]

in an extraction process

The fraction or percentage (R%) of the total quantity of a substance extracted (usually into the organic solvent phase) under specified conditions. Specifically, $R_{\mathrm{A}} = \frac{Q_{\mathrm{A}}}{(Q_{\mathrm{A}})'}$, where $(Q_{\mathrm{A}})'$ and Q_{A} are the original and final quantities of the substance A. This term is not recommended. Fraction extracted should be used.

Source:
Orange Book, p. 90
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2385

recrystallization

1. (chemical): The repeated dissolution and precipitation of a solid from a liquid solvent.
2. (metallurgical): The process in which a crystalline solid with a high degree of disorder develops a new microstructure by the nucleation of relatively imperfection-free regions, and their propagation throughout the complete solid.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 589

red shift

Informal term for bathochromic shift.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2270

redox ion exchangers

Conventional ion exchangers in which reversible redox couples have been introduced as counter-ions either by sorption or complex formation. They closely resemble redox polymers in their behaviour.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 855

redox polymer

Also contains definitions of: electron-exchange polymer, oxidation-reduction polymer

Polymer containing groups that can be reversibly reduced or oxidized.
Notes:

1. Reversible redox reaction can take place in a polymer main-chain, as in the case of polyaniline and quinone/hydroquinone polymers, or on side-groups, as in the case of a polymer carrying ferrocene side-groups.
2. Use of the term 'redox resin' is strongly discouraged.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 897

redox potential

Any oxidation-reduction (redox) reaction can be divided into two half reactions: one in which a chemical species undergoes oxidation and one in which another chemical species undergoes reduction. If a half- reaction is written as a reduction, the driving force is the reduction potential. If the half-reaction is written as oxidation, the driving force is the oxidation potential related to the reduction potential by a sign change. So the redox potential is the reduction/oxidation potential of a compound measured under standards conditions against a standard reference half-cell. In biological systems the standard redox potential is defined at pH – 7.0 versus the hydrogen electrode and partial pressure of hydrogen = 1 bar.
See also: electrode potential

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1294

reduced adsorption

Of component i, defined by the equation

$$\Gamma_i^{(n)} = \Gamma_i^{\sigma} - \Gamma_i \frac{c_i^{\alpha} - c_i^{\beta}}{c^{\alpha} - c^{\beta}}$$

where Γ^{σ}, c^{α} and c^{β} are, respectively, the total Gibbs surface concentration and the total concentrations in the bulk phases α and β:

$$\Gamma^{\sigma} = \sum_i \Gamma_i^{\sigma}$$

$$c^{\alpha} = \sum_i c_i^{\alpha}$$

$$c^{\beta} = \sum_i c_i^{\beta}$$

The reduced adsorption is invariant to the location of the Gibbs surface. Alternatively, the reduced adsorption may be regarded as the Gibbs surface concentration of i when the Gibbs surface is chosen so that Γ^{σ} is zero, i.e. the Gibbs surface is chosen so that the reference system has not only the same volume, but also contains the same total amount of substance (n) as the real system.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 591

reduced limiting sedimentation coefficient

See: sedimentation coefficient

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 617

reduced mass, μ

Effective mass in equations of motion for a many particle system.

Source:
Green Book, 2nd ed., p. 12

reduced mobile phase velocity, v

in chromatography

A term used mainly in liquid chromatography. It compares the mobile phase velocity with the velocity of diffusion into the pores of the particles (the so-called diffusion velocity, u_{D}):

$$v = \frac{\bar{u}}{u_{\mathrm{D}}} = \frac{\bar{u}\, d_{\mathrm{p}}}{D_{\mathrm{M}}}$$

In open-tubular chromatography:

$$v = \frac{\bar{u}\, d_{\mathrm{c}}}{D_{\mathrm{M}}}$$

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 840

reduced osmotic pressure

The osmotic pressure divided by mass concentration.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 615

reduced sample

A representative part of the primary (composited or gross) sample obtained by a division and reduction process. Typically the mass approximates that of the final laboratory sample.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1205

reduced sedimentation coefficient

See: sedimentation coefficient

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 617

reduced species

A term used to characterize the degree of reduction (or oxidation) in atoms, molecules and ions. An atom in a molecule or an ion which has a low oxidation state. An element or atom in a compound can be reduced by the reaction of an element or compound with hydrogen, while it can be oxidized by reaction with oxygen. A reduced species can be formed also through the gain of electrons (either at the negative electrode in a cell or through transfer from another atom, ion or group of atoms in a chemical reaction). For example, the carbon atom in CH_4 and other hydrocarbons is in a reduced state, while the carbon in CO_2 is in an oxidized state. Similarly the sulfur atom in H_2S is in a reduced state while that in sulfuric acid (H_2SO_4) is in an oxidized state.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2210

reduced viscosity

Synonym: viscosity number
of a polymer

of a polymer

The ratio of the relative viscosity increment to the mass concentration of the polymer, c, i.e. $\frac{\eta_i}{c}$, where η_i is the relative viscosity increment.

Notes:

1. The unit must be specified; $cm^3\ g^{-1}$ is recommended.
2. This quantity is neither a viscosity nor a pure number. The term is to be looked on as a traditional name. Any replacement by consistent terminology would produce unnecessary confusion in the polymer literature. Synonymous with viscosity number.

Source:
Purple Book, p. 63

reducing

in analytical chemistry

Decreasing the size of the laboratory sample or individual particles, or both. Division of the size of the laboratory sample may be accomplished manually by coning and quartering or by riffling or mechanically by rotary dividers. Reduction of particle size may be accomplished by milling or grinding. Simultaneous division and reduction may also be achieved with mills having stream diverters.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1204

reduction

The complete transfer of one or more electrons to a molecular entity (also called 'electronation'), and, more generally, the reverse of the processes described under oxidation (2) and (3).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1160

reductive elimination

The reverse of oxidative addition.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1160

reductones

Compounds containing an enediol structure stabilized by conjugation and hydrogen bonding with an adjacent carbonyl group, RC(OH)=C(OH)C(=O)R. They are strong reducing agents, fairly strong acids and commonly derived from saccharides by oxidation at the carbon atom alpha to the carbonyl function, e.g. ascorbic acid.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1363

referee sample

See: umpire sample

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1203

reference atom

in organic reaction mechanisms

The atom to which a primitive change is nucleophilic, electrophilic, nucleofugal or homolytic.

Source:
PAC, 1989, *61*, 23 *(System for symbolic representation of reaction mechanisms (Recommendations 1988))* on page 55

reference dose (RfD)

An estimate (with uncertainty spanning perhaps an order of magnitude) of daily exposure to the human population (including sensitive subgroups) that is likely to be without appreciable risk of deleterious effects during a lifetime.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1023

reference electrode

1. An external electrode system which comprises an inner element, usually mercury–mercury(I) chloride (calomel), silver–silver chloride or thallium amalgam–thallium(I) chloride, a chamber containing the appropriate filling solution and a device for forming a liquid junction, e.g. capillary, ceramic plug, fritted disc or ground glass sleeve.

   Source:
   Orange Book, p. 27
2. An electrode that maintains a virtually invariant potential under the conditions prevailing in an electrochemical measurement, and that serves to permit the observation, measurement, or control of the potential of the indicator (or test) or working electrode.

Source:
Orange Book, p. 60

See also:
Orange Book, p. 65

PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2533

reference material

A substance or mixture of substances, the composition of which is known within specified limits, and one or more of the properties of which is sufficiently well established to be used for the calibration of an apparatus, the assessment of a measuring method or for assigning values to materials. Reference materials are available from national laboratories in many countries [e.g. National Institute for Standards and Technology (NIST), USA.; Community Bureau of Reference, UK].

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2210

reference method

A method having small, estimated inaccuracies relative to the end use requirement. The accuracy of a reference method must be demonstrated through direct comparison with a definitive method or with a primary reference material.

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1702

reference procedure

in analysis of trace air constituents

Agreed method for determining one or more air quality characteristics where it is not practical to produce a reference material; the result obtained is defined as the measure of the air quality characteristic. For example, a gas such as NO_2 may be somewhat unstable when stored in a tank at low mixing ratios, so that the use of a more stable NO standard mixture in N_2 may be oxidized to NO_2 by O_3 in a specified manner referred to as the NO_2 reference procedure.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2210

reference state

of an element

The state in which the element is stable at a chosen standard-state pressure and for a given temperature.

Source:
PAC, 1982, *54*, 1239 *(Notation for states and processes, significance of the word standard in chemical thermodynamics, and remarks on commonly tabulated forms of thermodynamic functions)* on page 1249

reference value pH standard

An aqueous solution of 0.05 mol potassium hydrogen phthalate per kg water which is the reference value for the definition of pH(RVS) values in the temperature range $0\text{-}95\ °\text{C}$.
See also: operational pH standard, primary pH standard

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 540

reflectance, ρ

Also contains definitions of: reflectance factor, reflectivity

Fraction of incident radiation reflected by a surface or discontinuity, $\rho(\lambda) = \frac{P_\lambda^{\text{refl}}}{P_\lambda^0}$, where P_λ^0 and P_λ^{refl} are, respectively, the incident and reflected spectral radiant power.
Note:
The reflectance for a beam of light normally incident on a surface separating two materials of refractive indices n_1 and n_2 is given by

$$\rho(\lambda) = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2}$$

Reflectance increases as the angle of incidence decreases from 90 degrees.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 413

reflection electron energy loss spectroscopy (REELS)

Any technique in which a specimen is bombarded with a focused low energy ($E_0 < 10 \text{ eV}$) electron beam and the energy distribution of the reflected electrons is measured. This energy distribution contains features corresponding to discrete losses of energy of the reflected electrons due to excitation of vibrational and plasmon states and provides information on the type and geometric structure of compounds at the surface of the specimen.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2025

reflection factor

See: reflectance

Source:
Green Book, 2nd ed., p. 32

reflection high energy electron diffraction (RHEED)

Any technique which measures the angular intensity distribution of electrons 'reflected' from a crystalline surface under bombardment with high energy electrons near grazing incidence. The diffraction pattern provides very surface sensitive information (information depth $1\ \mathrm{nm}$) on the atomic arrangement of the top layers of a solid.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2025

refraction effects

The luminescence flux emitted from the interior of a rectangular sample reaching a photodetector place at some distance from the sample is decreased by a factor of approximately n^2 (where n is the refractive index of the medium) compared with a medium whose refractive index is 1.0. Such effects are termed refraction effects.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 244

refractive index, *n*

The ratio of the speed of light in vacuum to that in a given medium.

Source:
Green Book, 2nd ed., p. 30
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 989

refractive index increment

in polymer chemistry

The change of the solution refractive index, n, with solute concentration, C, i.e. $\frac{\partial n}{\partial C}$.
Notes:

1. The solute concentration is most frequently expressed in terms of mass concentration, molality or volume fraction. If expressed in terms of mass concentration or molality, the corresponding refractive index increments are referred to as specific or molal refractive index increments, respectively.
2. Following use of the full name, the abbreviated name refractive increment may be used.

Source:
Purple Book, p. 65

regeneration

of a catalyst

Reversal of catalytic deactivation with restoration of the original catalytic activity.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 84

regioselectivity (regioselective)

A regioselective reaction is one in which one direction of bond making or breaking occurs preferentially over all other possible directions. Reactions are termed completely (100%) regioselective if the discrimination is complete, or partially (x%), if the product of reaction at one site predominates over the product of reaction at other sites. The discrimination may also semi-quantitatively be referred to as high or low regioselectivity. (Originally the term was restricted to addition reactions of unsymmetrical reagents to unsymmetrical alkenes.) In the past, the term 'regiospecificity' was proposed for 100% regioselectivity. This terminology is not recommended owing to inconsistency with the terms stereoselectivity and stereospecificity.
See also: chemoselectivity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1160

regresssion analysis

Regression analysis is the use of statistical methods for modeling a set of dependent variables, Y, in terms of combinations of predictions, X. It includes methods such as multiple linear regression (MLR) and partial least squares (PLS).

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1149

regular block

in a polymer

A block that can be described by only one species of constitutional repeating unit in a single sequential arrangement.

Source:
Purple Book, p. 17

regular coke

A petroleum coke with good graphitizability, characterized by a combination of properties which differ significantly from those of metallurgical coke but do not reach the quality level of premium coke. These properties are: optical anisotropy, medium reversible thermal expansion and low ash content. Regular coke is mainly used for the production of synthetic carbon and graphite materials.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 503

regular macromolecule

A macromolecule the structure of which essentially comprises the repetition of a single constitutional unit with all units connected identically with respect to directional sense.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2289

regular oligomer molecule

An oligomer molecule the structure of which essentially comprises the repetition of a single constitutional unit with all units connected identically with respect to directional sense.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2290

regular polymer

A polymer composed of regular macromolecules, regular star macromolecules or regular comb macromolecules. A polymer consisting of star macromolecules with arms identical with respect to constitution and degree of polymerization is considered to be regular; ***See:*** star macromolecule, [note 2]. Analogously, a polymer consisting of comb macromolecules with the sub-chains between the branch points of the main chain and the terminal sub-chains of the main chain identical with respect to constitution and degree of polymerization and the side-chains identical with respect to constitution and degree of polymerization is considered to be regular; ***See:*** comb macromolecule, [note 1].

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2302

regular single-strand polymer

A regular linear polymer that can be described by a preferred constitutional repeating unit in which both terminal constituent subunits are connected through single atoms to the other identical constitutional repeating units or to an end group.

Source:
Purple Book, p. 110

regulator gene

A gene which codes for a protein (an activator of repressor) having the ability to induce or repress the transcription of other genes.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 164

Rehm–Weller equation

Empirical correlation found between the observed second-order rate constant, k_{q}, for an intermolecular electron-transfer reaction and the Gibbs energy of the photoinduced electron transfer process within the encounter complex ($\Delta_{\mathrm{ET}}G^{\mathrm{o}}$):

$$k_{\mathrm{q}} = \frac{k_{\mathrm{d}}}{1 + \frac{k_d}{K_{\mathrm{d}} Z}\left[\exp\left(\frac{\Delta G^{\ddagger}}{R\,T}\right) + \exp\left(\frac{\Delta_{\mathrm{ET}} G^{\mathrm{o}}}{R\,T}\right)\right]}$$

with k_{d} and $k_{-\mathrm{d}}$ the rate constant for the formation and separation, respectively, of the encounter (precursor) complex, $K_{\mathrm{d}} = {}^{k_{\mathrm{d}}}\!/_{k_{-\mathrm{d}}}$, Z the universal collision frequency factor, R the gas constant, T the absolute temperature and $\Delta G^{\ddagger}$ the activation Gibbs energy of the forward electron transfer reaction.
Note:
In the original formulation of this equation the value $\frac{k_d}{K_{\mathrm{d}} Z} = 0.25$ in acetonitrile was used.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 413

reinforced reaction injection moulding

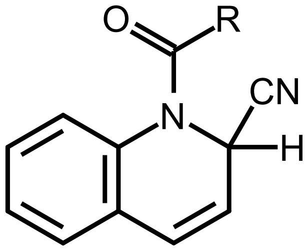
Acronym: RRIM

Reaction injection moulding within which glass fibres are included to increase the strength of the moulding.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1825

Reissert compounds

Compounds formed by formal addition of an acyl group and a cyano group to a nitrogen atom and carbon atom, respectively, of a nitrogen–carbon bond in quinolines, isoquinolines, and related nitrogen heterocycles, e.g.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1363

rel

See: relative configuration

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2216

relative

Quotient of quantities having the same kind-of-quantity in different systems.
Notes:
1. The denominator quantity is often called the reference quantity.
2. Preferentially the same component is found in the numerator and denominator quantity.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 989

relative activity

See: activity

Source:
Green Book, 2nd ed., p. 49
Green Book, 2nd ed., p. 22

relative adsorption

If Γ_i^σ and Γ_1^σ are the Gibbs surface concentrations of components i and 1, respectively, with reference to the same, but arbitrarily chosen, Gibbs surface, then the relative adsorption of component i with respect to component 1, is defined as

$$\Gamma_i^{(1)} = \Gamma_i^\sigma - \Gamma_1^\sigma \frac{c_i^\alpha - c_i^\beta}{c_1^\alpha - c_1^\beta}$$

and is invariant to the location of the Gibbs surface. Alternatively, $\Gamma_i^{(1)}$ may be regarded as the Gibbs surface concentration of i when the Gibbs surface is chosen so that Γ_i^σ is zero, i.e. the Gibbs surface is chosen so that the reference system contains the same amount of component 1 as the real system. Hence $\Gamma_1^{(1)} \equiv 0$.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 591

relative atomic mass (atomic weight), A_r

The ratio of the average mass of the atom to the unified atomic mass unit.
See also: standard atomic weight

Source:
Green Book, 2nd ed., p. 41
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 990

relative biological effectiveness

of radiation

The ratio of the appropriate value of the biological effectiveness of the radiation in question to that of X-radiation with an average specific ionization of 100 ion pairs per micron of water, for the particular biological effect under consideration and for the condition under which the radiation is received.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1551

relative configuration

1. The configuration of any stereogenic (asymmetric) centre with respect to any other *stereogenic* centre contained within the same molecular entity. Unlike absolute configuration, relative configuration is reflection-invariant. Relative configuration, distinguishing diastereoisomers, may be denoted by the configurational descriptors R^*, R^* (or *l*) and R^*, S^* (or *u*) meaning,

respectively, that the two centres have identical or opposite configurations. For molecules with more than two asymmetric centres the prefix *rel*- may be used in front of the name of one enantiomer where *R* and *S* have been used. If any centres have known absolute configuration then only R^* and S^* can be used for the relative configuration.
See also: α (alpha), β (beta) (1 and 3)

2. Two different molecules Xabcd and Xabce, may be said to have the same relative configurations if e takes the position of d in the tetrahedral arrangement of ligands around X (i.e. the pyramidal fragments Xabc are superposable). By the same token the enantiomer of Xabce may be said to have the opposite relative configuration to Xabcd. The terms may be applied to chiral molecular entities with central atoms other than carbon but are limited to cases where the two related molecules differ in a single ligand.
   Both definitions can be generalized to include stereogenic units other than asymmetric centres.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2217

relative counting

in nuclear chemistry

A measurement in which the activity of a test portion is derived from the ratio between the count rates observed for the test portion and for a radioactive source of known activity.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

relative density, *d*

Ratio of density to a reference density, usually the density of water at 4 °C; in the older literature this is called specific gravity.

Source:
Green Book, 2nd ed., p. 12
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2210

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 990

relative detection limit

(Often incorrectly referred to as sensitivity). Smallest amount of material detectable (3σ-criterion) in a matrix relative to the amount of material analysed — given in atomic, mole or weight fractions.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

relative electrode potential

The electrode potential of a single electrode is not amenable to direct experimental determination and can only be measured against a reference system. The measured quantity, E, is the relative electrode potential.

Source:
PAC, 1986, *58*, 955 *(The absolute electrode potential: an explanatory note (Recommendations 1986))* on page 956

relative elongation

See: linear strain

Source:
Green Book, 2nd ed., p. 12

relative error

Error of measurement divided by the true value of the measurand. Since a true value cannot be determined, in practice the conventional true value is used.

Source:
VIM

See also:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 601

relative hardness

The difference between the values of the absolute hardnesses (η) of a given molecule and the corresponding reference structure (η_a): $\eta_r = \eta - \eta_a$. The values of relative hardnesses correlate well with the resonance energies of cyclic compounds and may be used as an index of aromaticity.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1960

relative humidity

The ratio, often expressed as a percentage, of the partial pressure of water in the atmosphere at some observed temperature, to the saturation vapour pressure of pure water at this temperature.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2210

relative micellar mass

Also contains definition of: micellar weight

The relative molecular mass (M_r) of a micelle is called the relative micellar mass or micellar weight and is defined as the mass of a mole of micelles divided by the mass of $\frac{1}{12}$ mole of ^{12}C.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

relative molar mass

Molar mass divided by 1 g mol^{-1} (the latter is sometimes called the standard molar mass).

Source:
Green Book, 2nd ed., p. 41

relative molecular mass, M_r

Ratio of the mass of a molecule to the unified atomic mass unit. Sometimes called the molecular weight or relative molar mass.

Source:
Green Book, 2nd ed., p. 41
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 990

relative permeability, μ_r

Ratio of the magnetic flux density in a given medium to that in vacuum.

Source:
Green Book, 2nd ed., p. 15

relative permittivity, ε_r

Ratio of the electric field strength in vacuum to that in a given medium. It was formerly called the dielectric constant.

Source:
Green Book, 2nd ed., p. 14

relative preconcentration

in trace analysis

An operation (process) as a result of which the ratio of concentration or amounts of microcomponents and main macrocomponents increases. This is a particular example of a separation, but at greatly differing concentrations of components. The ratio of the masses of the initial and final samples is not of great importance. Frequently, the main purpose of relative preconcentration is the replacement of a matrix unsuitable for analysis by a suitable medium. In some cases, it is difficult to trace a boundary between the absolute and the relative preconcentrations as, for example, in preconcentration by zone melting.

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1197

relative retardation, R_{rel}

in planar chromatography

A term which is equivalent to relative retention used in column chromatography: the ratio of the R_{F} value of a component to the R_{F} value of a standard (reference) substance. Since the mobile phase front is common for the two components, the R_{F} value can be expressed directly as the ratio of the distances travelled by the spot of the compound of interest (b_i) and the reference substance (b_{st}) respectively:

$$R_{\mathrm{rel}} = \frac{R_{\mathrm{F}(i)}}{R_{\mathrm{F(st)}}} = \frac{b_i}{b_{\mathrm{st}}}$$

In former nomenclatures the symbol R_{s} was used to express relative retardation in planar chromatography. Because of its identity with the symbol for peak resolution the symbol R_{rel} is suggested for relative retardation in planar chromatography.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 845

relative retention, r

in column chromatography

The ratio of the adjusted or net retention volume (time) or retention factor of a component relative to that of a standard, obtained under identical conditions:

$$r = \frac{V'_{\mathrm{R}i}}{V'_{\mathrm{R(st)}}} = \frac{V_{\mathrm{N}i}}{V_{\mathrm{N(st)}}} = \frac{t'_{\mathrm{R}i}}{t'_{\mathrm{R(st)}}} = \frac{k_i}{k_{\mathrm{st}}}$$

Depending on the relative position of the peak corresponding to the standard compound in the chromatogram, the value of r may be smaller, larger or identical to unity.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 843
Orange Book, p. 105

relative selectivity

in catalysis

See: fractional selectivity *in catalysis*

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 81

relative spectral responsivity

See: action spectrum, responsivity

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2270
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1749

relative standard deviation, s_{r}, σ_{r}

The standard deviation divided by the mean of the series. It can be calculated with the formula:

$$s_{\mathrm{r}} = \frac{s}{\bar{x}}$$

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 601
Orange Book, p. 5

relative uncertainty

Uncertainty divided by the mean value.

Source:
VIM

relative viscosity

Synonym: viscosity ratio

The ratio of the viscosity of the solution, η, to the viscosity of the solvent, η_s, i.e. $\eta_r = \frac{\eta}{\eta_s}$. Synonymous with viscosity ratio.

Source:
Purple Book, p. 62

relative viscosity increment

The ratio of the difference between the viscosities of solution and solvent to the viscosity of the solvent, i.e. $\eta_i = \frac{\eta - \eta_s}{\eta_s}$, where η is the viscosity of the solution and η_s is the viscosity of the solvent. The use of the term 'specific viscosity' for this quantity is discouraged, since the relative viscosity increment does not have the attributes of a specific quantity.

Source:
Purple Book, p. 63

relative volumic mass

Synonymous with relative density.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2472

relativistic effects

Corrections to exact non-relativistic energy from the fact that inner shell electrons in heavy atoms move with velocities comparable in order of magnitude to the velocity of light. The most important relativistic effect is spin-orbit coupling.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1960

relaxation

If a system is disturbed from its state of equilibrium it relaxes to that state, and the process is referred to as relaxation. The branch of kinetics concerned with such processes is known as relaxation kinetics. Relaxation techniques include temperature jump and pressure jump.
See also: chemical relaxation

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 185
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1160

PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2297

relaxation kinetics

See: relaxation

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 185
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1160
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2297

relaxation time

1. In magnetic resonance spectroscopy the longitudinal relaxation time, T_1, is associated with spin-lattice relaxation, and the transverse relaxation time, T_2, with spin-spin relaxation. The definitions are: $\frac{\mathrm{d}M_z}{\mathrm{d}t} = -\frac{M_z - M_{z,\mathrm{e}}}{T_1}$ and $\frac{\mathrm{d}M_x}{\mathrm{d}t} = -\frac{M_x}{T_2}$, where M_z and M_x are the components of magnetization parallel and perpendicular to the static field B and the subscript e denotes the equilibrium value.

   Source:
   Green Book, 2nd ed., p. 25
2. In a chemical reaction, the time, τ, in which a concentration perturbation falls to $\frac{1}{\mathrm{e}}$ of its initial value.

Source:
Green Book, 2nd ed., p. 55

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 185

releaser

in analytical flame spectroscopy

A substance which reduces solute-volatilization interferences by forming a compound preferentially with the interferent, thus preventing the reaction of the analyte or interferent from entering a thermally stable compound.

Source:
Orange Book, p. 172

rem

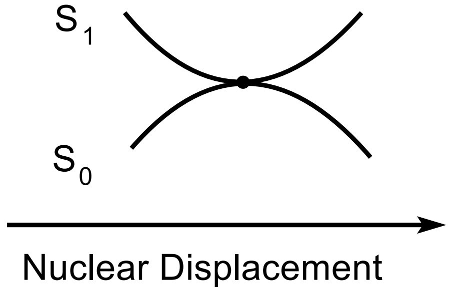
Non-SI unit of dose equivalent ($\mathrm{rem} = 0.01\ \mathrm{Sv}$).

Source:
Green Book, 2nd ed., p. 113
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 990

Renner–Teller effect

Molecular distortion in linear molecular species with degenerate electronic states (e.g., belonging to the $C_{\infty v}$ group). The Renner–Teller effect is a particular case of the Jahn–Teller effect. From the point of view of the potential? energy surfaces the Renner–Teller effect generates a surface touching (see scheme below).
Notes:

1. The Renner–Teller effect arises from splittings in the vibrational levels of molecular entities due to even terms in the vibronic perturbation expansion. This is generally a minor effect for non-linear molecular entities compared to the Jahn–Teller effect, which is due to the odd terms.
2. For linear molecular entities it is the only possible vibronic effect characteristic of degenerate electronic states.



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 414

reorganization energy

in electron transfer

Gibbs energy dissipated when a system that has undergone 'vertical' electron transfer (i.e., electron transfer obeying the Franck–Condon principle) relaxes to the equilibrium state for its new charge distribution. Commonly the total reorganization energy (λ) is written as the sum of an inner contribution (λ_{in}) and an outer contribution (λ_{out}) attributed to nuclear reorganizations of the redox partners and their environment (solvent), respectively.
Note:
Approximations have been proposed to calculate the value of λ_{out} taking into account the 'relative permittivity' of the solvent.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 414

reorganization

in polymers

The molecular process by which (i) amorphous or poorly ordered regions of a polymer specimen become incorporated into crystals, or (ii) a change to a more stable crystal structure takes place, or (iii) defects within the crystal decrease.
Notes:
1. Secondary crystallization may be involved in the reorganization process.
2. Reorganization may result from annealing.
3. Points (i) and (ii) above may also be called crystal perfection.

Source:
Purple Book, p. 85

repeatability

The closeness of agreement between independent results obtained with the same method on identical test material, under the same conditions (same operator, same apparatus, same laboratory and after short intervals of time). The measure of repeatability is the standard deviation qualified with the term: `repeatability' as repeatability standard deviation. In some contexts repeatability may be defined as the value below which the absolute difference between two single test results obtained under the above conditions, may be expected to lie with a specified probability.
See also: reproducibility

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 598

See also:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1701
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2210

repetency

See: wavenumber

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 990

replacement name

A name in which the replacement of an atom or a group of a parent structure by another atom or group is indicated by affixes attached to or inserted into the name of the parent structure. There are two main types of replacement names.

1. Skeletal replacement name. A name in which the replacement of skeletal atoms and their associated hydrogen atoms is indicated by non-detachable prefixes. When carbon atoms are replaced by heteroatoms this method has been called 'a' nomenclature since the prefixes end in 'a'. Certain names in which the prefix 'thio-', 'seleno-' or 'telluro-' indicates replacement of a skeletal oxygen atom by a sulfur, selenium or tellurium atom, respectively, are also skeletal replacement names.
2. Functional replacement name. A name containing prefixes or infixes which indicate the replacement of an oxygen atom or hydroxy group of a characteristic group, functional parent or class name by other atoms or groups.

Source:
Blue Book (Guide), p. 15

replacement operation

in organic nomenclature

The exchange of one group of atoms or a single non-hydrogen atom for another.

Source:
Blue Book (Guide), p. 23

replicate (duplicate) sample

Multiple (or two) samples taken under comparable conditions. This selection may be accomplished by taking units adjacent in time or space. Although the replicate samples are expected to be identical, often the only thing replicated is the act of taking the physical sample. A duplicate sample is a replicate sample consisting of two portions. The umpire sample is usually used to settle a dispute; the replicate sample is usually used to estimate sample variability.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1203

replication

The duplication of DNA as part of the reproductive cycle of a cell or virus. During replication the two DNA strands in the double helix separate, and each strand then acts as a template specifying the base sequence of newly synthesized complementary strands.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 164

report

in analysis

A combination of specimen information and results. The report should contain information about unequivocal identification of the source and type of material analysed and the requesting agency. It may contain such other information that is pertinent to the correct interpretation of a result (e.g. confidence interval, reference data and interpretative information).

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1659

reprecipitation

The planned repetition of a precipitation in order to remove chemically different species from a previous precipitate or to improve its stoichiometry.

Source:
Orange Book, p. 86

representative sample

A sample resulting from a sampling plan that can be expected to adequately reflect the properties of interest of the parent population. A representative sample may be a random sample or, for example, a stratified sample, depending upon the objective of sampling and the characteristics of the population. The degree of representativeness of the sample may be limited by cost or convenience.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1202

repression

Binding of a protein (repressor) to the operator sequence in an operon thus preventing the transcription of the following structural gene(s) into mRNA and consequently synthesis of protein (cf. enzyme repression).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 164

reproducibility

The closeness of agreement between independent results obtained with the same method on identical test material but under different conditions (different operators, different apparatus, different laboratories and/or after different intervals of time). The measure of reproducibility is the standard deviation qualified with the term 'reproducibility' as reproducibility standard deviation. In some contexts reproducibility may be defined as the value below which the absolute difference between two

single test results on identical material obtained under the above conditions, may be expected to lie with a specified probability. Note that a complete statement of reproducibility requires specification of the experimental conditions which differ.
See also: repeatability

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 598

See also:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1707
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2210

repulsive potential-energy surface

Also contains definition of: late-downhill surface

A surface for an exergonic reaction A + BC in which the col corresponds to considerable separation between the products A–B + C . The energy barrier in the potential-energy profile is in the later stages of the reaction path. On such a surface most of the energy is released after A–B is formed. Repulsive surfaces are also called late-downhill surfaces, and the barrier in such a surface is called a Type-II barrier.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 185

reserve sample

See: umpire sample

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1203

residence time

1. (instrumentation): The time required for air or reagent parcel to pass from the entrance to the exit of an instrument. Often this is approximated as the ratio of the interior volume of the device to the flow rate.
2. (atmospheric): The average time a molecule or aerosol spends in the atmosphere after it is released or generated there. For compounds with well defined sources and emission rates, this is estimated by the ratio of the average global concentration of a substance to its production rate on a global scale. It is a function of not only the emission rates but the loss rates by chemical and physical removal processes.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2211

residence time (hydraulic retention time), t_r

in biotechnology

The average time a particle or volume element of the culture resides in a bioreactor (or other device) through which a liquid medium continously flows. Residence time of the liquid is the reciprocal of dilution rate.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 164

residual current

The current that flows, at any particular value of the applied potential, in the absence of the substance whose behaviour is being investigated (i.e. in a blank solution).

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1499

residual emission anisotropy

Photoselected molecules hindered in their rotation (e.g., in lipid bilayers or liquid crystals) do not become randomly oriented even after long time periods. Thus, the emission anisotropy does not decay to zero but to a steady value, r_∞, called residual emission anisotropy. In the case of a single rotational correlation time, τ_c or θ, the decay of emission anisotropy following δ-pulse excitation is given by:

$$r(t) = \left(r_0 - r_\infty\right) \exp\left(-\frac{t}{\tau_c}\right) + r_\infty$$

where r_0 is the fundamental emission anisotropy.
Note:
The term residual anisotropy is to be preferred to 'limiting anisotropy'.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 414

residual fuel/oil

The liquid or semi-liquid, high-boiling fraction of residue from the distillation of petroleum which is used as a fuel. After removal of the lower boiling fraction of crude oil, sold as petroleum gas, the somewhat higher boiling fraction becomes gasoline and diesel oil. A portion of the higher boiling fraction is 'cracked' to yield additional gasoline. Still heavier oils become lubricants. Paraffin, asphalt, etc., are also extracted from the crude oil. It is the remaining residual oil, not economically usable for other industrial purposes, which is then sold as a relatively low cost fuel for burning.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2211

residual liquid junction (potential) error

in pH measurement

Error arising from breakdown in the assumption that the liquid junction potential remains constant when solution X is substituted for solution S in the operational cell.

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 541

residual spectrum/background spectrum

in mass spectrometry

Set of peaks recorded in the absence of a sample and due either to small air leaks or to the presence of molecules desorbed from the walls of the introduction device or the source, or from the pump fluid.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2211

resin

Soft solid or highly viscous substance, usually containing prepolymers with reactive groups.
Notes:

1. This term was used originally because of its analogy with a natural resin (rosin) and designated, in a broad sense, any polymer that is a basic material for plastics, organic coatings, or lacquers. However, the term is now used in a more narrow sense to refer to prepolymers of thermosets (thermosetting polymers).
2. The term is sometimes used not only for prepolymers of thermosets, but also for cured thermosets (e.g., epoxy resins, phenolic resins). Use of the term for cured thermosets is strongly discouraged.
3. Use of the term 'resin' to describe the polymer beads used in solid-phase synthesis and as polymer supports, catalysts, reagents, and scavengers is also discouraged.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 897

resist polymer

Polymeric material that, when irradiated, undergoes a marked change in solubility in a given solvent or is ablated.
Notes:

1. A resist polymer under irradiation either forms patterns directly or undergoes chemical reactions leading to pattern formation after subsequent processing.
2. A resist material that is optimized for use with ultraviolet or visible light, an electron beam, an ion beam, or X-rays is called a photoresist, electron-beam resist, ion-beam resist, or X-ray resist, respectively.
3. In a positive-tone resist, also called a positive resist, the material in the irradiated area not covered by a mask is removed, which results in an image with a pattern identical with that on the mask. In a negative-tone resist, also called a negative resist, the non-irradiated area is subsequently removed, which results in an image with a pattern that is the complement of that on the mask.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 903

resistance, R

Electric potential difference divided by the electric current when there is no electromotive force in a conductor.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 990

resistivity, ρ

Electric field strength divided by the current density. This quantity is a tensor in an anisotropic medium.

Source:
Green Book, 2nd ed., p. 15
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 990

resolution

in gas chromatography

A characteristic of the separation of two adjacent peaks. It may be expressed according to the equation:

$$R_{\mathrm{AB}} = 2\,\frac{|\,d_{\mathrm{R}}(\mathrm{B}) - d_{\mathrm{R}}(\mathrm{A})\,|}{|\,w(\mathrm{B}) + w(\mathrm{A})\,|}$$

where R_{AB} is the resolution, $d_{\mathrm{R}}(\mathrm{A})$ and $d_{\mathrm{R}}(\mathrm{B})$ are the retention distances (time or volume) of each eluted component A and B, and $w(\mathrm{A})$ and $w(\mathrm{B})$ are the respective widths of each peak at its base.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2211

resolution

in mass spectroscopy

1. (energy): By analogy with the peak width definition for mass resolution, a peak showing the number of ions as a function of their translational energy should be used to give a value for the energy resolution.
2. (10 per cent valley definition): Let two peaks of equal height in a mass spectrum at masses m and $m - \Delta m$ be separated by a valley which at its lowest point is just 10 per cent of the height of either peak. For similar peaks at a mass exceeding m, let the height of the valley at its lowest point be more (by any amount) than ten per cent of either peak height. Then the resolution (10 per cent valley definition) is $\frac{m}{\Delta m}$. It is usually a function of m. The ratio $\frac{m}{\Delta m}$ should be given for a number of values of m.
3. (peak width definition): For a single peak made up of singly charged ions at mass m in a mass spectrum, the resolution may be expressed as $\frac{m}{\Delta m}$ where Δm is the width of the peak at a height which is a specified fraction of the maximum peak height. It is recommended that one of three values 50%, 5% or 0.5% should always be used. For an isolated symmetrical peak recorded with a system which is linear in the range between 5% and 10% levels of the peak, the 5% peak width definition is technically equivalent to the 10% valley definition. A common standard is the definition of resolution based upon Δm being Full Width of the peak at Half its Maximum height, sometimes abbreviated 'FWHM'. This acronym should preferably be defined the first time it is used.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1554
Orange Book, p. 203

resolution

in optical spectroscopy

Wavenumber, wavelength or frequency difference of two still distinguishable lines in a spectrum.

Source:
Green Book, 2nd ed., p. 31

resolution

in stereochemistry

The separation of a racemate into the component enantiomers.
See also: kinetic resolution, racemic conglomerate

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2217

resolving power

in mass spectrometry

The ability to distinguish between ions differing in the quotient mass/charge by a small increment. It may be characterized by giving the peak width, measured in mass units, expressed as a function of mass, for at least two points on the peak, specifically at fifty percent and at five percent of the maximum peak height.

Source:
Orange Book, p. 203
PAC, 1978, *50*, 65 *(Recommendations for symbolism and nomenclature for mass spectroscopy)* on page 72
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1554

resolving power, R

in optical spectroscopy

Transition wavenumber (or wavelength or frequency) divided by the resolution.

Source:
Green Book, 2nd ed., p. 31

resolving time correction

in nuclear analytical chemistry

Correction to be applied to the observed number of pulses in order to take into account the number of pulses lost during the resolving time.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1551

resolving time

in nuclear analytical chemistry

The smallest time interval which must elapse between the occurrence of two consecutive ionizing events or signal pulses, in order that the measuring device be capable of fulfilling its function of each of them separately.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1551

resonance

In the context of chemistry, the term refers to the representation of the electronic structure of a molecular entity in terms of contributing structures. Resonance among contributing structures means that the wavefunction is represented by 'mixing' the wavefunctions of the contributing structures. The concept is the basis of the quantum mechanical valence bond methods. The resulting stabilization is linked to the quantum mechanical concept of 'resonance energy'. The term resonance is also used to refer to the delocalization phenomenon itself.
See also: mesomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1161

resonance absorption technique

The monitoring of atoms or radicals generated in the gas phase by observing the attenuation of the radiation from a lamp emitting the characteristic resonance radiation of the observed species.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2271

resonance cross-section
in Mössbauer spectrometry

The cross-section for resonant absorption of the Mössbauer transition γ ray.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 214

resonance effect magnitude
in Mössbauer spectrometry

Ratio of the difference in the transmitted or scattered intensity at resonance maximum and off-resonance, relative to the intensity off-resonance.

Source:
PAC, 1976, *45*, 211 *(Nomenclature and Conventions for Reporting Mossbauer Spectroscopic Data)* on page 214

resonance energy

The difference in potential energy between the actual molecular entity and the contributing structure of lowest potential energy. The resonance energy cannot be measured, but only estimated, since contributing structures are not observable molecular entities.
See: resonance

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1161

resonance energy

in radiochemistry

The energy of a particle entering a nuclear reaction, this energy being just sufficiently high to lead to the formation of reaction products in one of their excited states.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

resonance fluorescence

Fluorescence from the primary excited atomic or molecular species at the wavelength of the exciting radiation (no relaxation within the excited manifold). This term is also used to designate the radiation emitted by an atom of the same wavelength as the longest one capable of exciting its fluorescence, e.g. $122.6\ \mathrm{nm}$ in the case of the hydrogen atom, and $253.7\ \mathrm{nm}$ in the case of the mercury atom.
See also: resonance line *in photochemistry*

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2271

resonance fluorescence technique

The monitoring of atoms or radicals generated in the gas phase by observing the intensity of fluorescence (exitance) emitted by the species after excitation with radiation of the same wavelength.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2271

resonance hybrid

A localized valence bond representation of a molecule. This describes pictorially an electronic wavefunction that makes some contribution to the state wavefunction of the system. Resonance hybrids are needed to describe the state of a system when that system is not adequately described by a single Lewis structure.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1961

resonance integral, H_{rs}

In Hückel molecular orbital theory, the integral over space of the type $\int \psi_r^* \hat{H} \psi_s \mathrm{d}\tau$ where $\hat{H}$ is the hamiltonian operator and ψ_r and ψ_s are different wavefunctions.

Source:
Green Book, 2nd ed., p. 17

resonance integral

in radiochemistry

The integral, over all or some specified portion of the resonance energy range, of the cross-section divided by the energy of a radiation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

resonance lamp

Lamp emitting resonance radiation of atoms and their ions. Depending on the requirements, the lamp is filled either with pure vapour of the element or with a mixture of it and other gases.
Note:
Examples are: Hg (253.7 and 184.9 nm), Cd (228.8 and 643.8 nm), Na (589.0 nm), Zn (213.8, 330.3, 334.5, and 636.2 nm), Kr (116.5 and 123.6 nm), Xe (129.6 and 147.0 nm).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 415

resonance line

in photochemistry

The longest wavelength capable of exciting fluorescence in an atom.
See also: resonance fluorescence

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2271

resonance line

Also contains definition of: resonance emission

in X-ray spectroscopy

The radiative decay of an excitation level may proceed to the neutral ground state and would thus occur at the same energy as the corresponding line in the absorption spectrum. Such a line is called a resonance line and the process is called resonance emission.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 739

resonance neutrons

Neutrons whose energy corresponds to the resonance energy of a specified nuclide or element. If the nuclide is not specified, the term refers to resonance neutrons of ^{239}U.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

resonance radiation

Synonymous with resonance fluorescence.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2271

response constant

in electroanalytical chemistry

A quantity whose expression includes a current, whose value is characteristic of a charge-transfer process and the experimental conditions under which it is investigated, and whose nature depends on the technique that is employed. Some typical response constants are the diffusion current constant in polarography, the voltammetric constant in linear-sweep voltammetry, and the chronopotentiometric constant in chronopotentiometry.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1504

response time, τ_R

Also contains definition of: rise time *of a radiation detector*

of a detector

The time required for the detector output to go from the initial value to a percentage (e.g. 99%) of the final value. In the case of an exponential behaviour of the detector τ_R can be related to the time constant τ_c. The rise time τ_r is the time required for the detector output to vary between given percentages (e.g. from 10% to 90%) of the final value. Similarly, the fall time τ_f is the time required for the detector output to vary between given percentages (e.g. from 90% to 10%) of the initial value.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1751

response time

of an analyser

Time which elapses, when there is a stepwise change in the quantity to be measured, between the moment when this change is produced and the moment when the indication reaches a value conventionally fixed at 90% of the final change in indication.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

responsive gel

Gel that responds to external electrical, mechanical, thermal, light-induced or chemical stimulation.
Note:
The use of the term intelligent gel is discouraged.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1808

responsivity, *R*

Also contains definitions of: dark current, dark output, dark resistance, relative responsivity, spectral responsivity function, useful spectral range

in detection of radiation

Detector input can be e.g. radiant power, irradiation, radiant energy. It produces a measurable detector output which may be e.g. an electrical charge, an electrical current or potential or a change in pressure. The ratio of the detector output and the detector input is defined as the responsivity. It is given in e.g. ampere/watt, volt/watt. The responsivity is a special case of the general term sensitivity. Dark current is the term for the electrical output of a detector in the absence of input. This is a special case of the general term dark output. For photoconductive detectors the term dark resistance is used. If the responsivity is normalized with regard to that obtained from a reference radiation the resulting ratio is called relative responsivity. For measurements with monochromatic radiation at a given wavelength the term spectral responsivity $R(\lambda)$ is used. In some cases the relative spectral responsivity, where the spectral responsivity is normalized with respect to the responsivity at some given wavelength, is used. The dependence of the spectral responsivity on the wavelength is described by the spectral responsivity function. The useful spectral range of the detector should be given as the wavelength range where the relative responsivity does not fall below a specified value.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1749

rest point

of a balance

The position of the pointer with respect to the pointer scale when the motion of the beam has ceased.

Source:
Orange Book, p. 36

restriction enzymes

Endonucleases which recognize specific base sequences within a DNA helix, creating a double-strand break of DNA. Type I restriction enzymes bind to these recognition sites but subsequently cut the DNA at different sites. Type II restriction enzymes both bind and cut within their recognition or target sites.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 164

result

in analysis

The final value reported for a measured or computed quantity, after performing a measuring procedure including all subprocedures and evaluations.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 597

retardation factor, R

in column chromatography

The fraction of the sample component in the mobile phase at equilibrium; it is related to the retention factor and other fundamental chromatography terms:

$$R = \frac{1}{k + 1}$$

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 843

retardation factor, R_F

in planar chromatography

Ratio of the distance travelled by the centre of the spot to the distance simultaneously travelled by the mobile phase:

$$R_F = \frac{b}{a}$$

By definition the R_F values are always less than unity. They are usually given to two decimal places. In order to simplify this presentation the hR_F values may be used: they correspond to the R_F values multiplied by 100. Ideally, R_F values are identical to the R values used in column chromatography.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 845

retarder

This term, used mainly in polymerization kinetics, refers to a substance that reduces the rate of reaction. Synonymous with inhibitor.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 185

retentate

See: dialysate

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

retention efficiency

in particle separation

The ratio of the quantity of particles retained by a separator to the quantity entering it (generally expressed as a percentage).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2211

retention factor, k

in column chromatography

A measure of the time the sample component resides in the stationary phase relative to the time it resides in the mobile phase; it expresses how much longer a sample component is retarded by the stationary phase than it would take to travel through the column with the velocity of the mobile phase. Mathematically, it is the ratio of the adjusted retention volume (time) and the hold-up volume (time):

$$k = \frac{V_R'}{V_M} = \frac{t_R'}{t_M}$$

If the distribution constant is independent of sample component concentration, then the retention factor is also equal to the ratio of the amounts of a sample component in the stationary and mobile phases respectively, at equilibrium:

$$k = \frac{\text{amount of component in stationary phase}}{\text{amount of component in mobile phase}}$$

If the fraction of the sample component in the mobile phase is R, then the fraction in the stationary phase is $1 - R$; thus

$$k = \frac{1 - R}{R}$$

In former nomenclatures and in the literature one may find the expressions partition ratio, capacity ratio, capacity factor or mass distribution ratio to describe this term. In the literature the symbol k' is often used for the retention factor, particularly in liquid chromatography. The original reason for this was to clearly distinguish it from the partition coefficient (distribution constant) for which the symbol K had been utilized. Since, however, the distribution constants are all identified with a subscript, there is no reason to add the prime sign to this symbol. It should be emphasized that all the recognized nomenclatures (IUPAC, BS, ASTM) have always clearly identified the capacity factor with the symbol k and not k'. The logarithm of the retention factor is equivalent to the R_M value used in planar chromatography. The symbol κ is suggested to express

$$\kappa = \log_{10} k = \log_{10}\left[\frac{1 - R}{R}\right]$$

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 843

retention

in nuclear chemistry

Of atoms undergoing a nuclear transformation, that fraction which remains in or reverts to its initial chemical form.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1551

retention index, *I*

Also contains definition of: Kováts (retention) index

in column chromatography

The retention index of a sample component is a number, obtained by interpolation (usually logarithmic), relating the adjusted retention volume (time) or the retention factor of the sample component to the adjusted retention volumes (times) of two standards eluted before and after the peak of the sample component. In the Kováts index or Kováts retention index used in gas chromatography, *n*-alkanes serve as the standards and logarithmic interpolation is utilized:

$$I = 100\left[\frac{\log_{10} X_i - \log_{10} X_z}{\log_{10} X_{z+1} - \log_{10} X_z} + z\right]$$

where X refers to the adjusted retention volumes or times, z is the number of carbon atoms of the *n*-alkane eluting before and $(z+1)$ is the number of carbon atoms of the *n*-alkane eluting after the peak of interest:

$$V'_{\mathrm{R}\,z} < V'_{\mathrm{R}\,i} < V_{\mathrm{R}\,(z+1)}$$

The Kováts (retention) index expresses the number of carbon atoms (multiplied by 100) of a hypothetical normal alkane which would have an adjusted retention volume (time) identical to that of the peak of interest when analysed under identical conditions. The Kováts retention index is always measured under isothermal conditions. In the case of temperature-programmed gas chromatography a similar value can be calculated utilizing direct numbers instead of their logarithm. Since both the numerator and denominator contain the difference of two values, here we can use the total retention volumes (times). Sometimes this value is called the linear retention index.

$$I^{\mathrm{T}} = 100\left[\frac{t^{\mathrm{T}}_{\mathrm{R}\,i} - t^{\mathrm{T}}_{\mathrm{R}\,z}}{t^{\mathrm{T}}_{\mathrm{R}\,(z+1)} - t^{\mathrm{T}}_{\mathrm{R}\,z}} + z\right]$$

where $t^{\mathrm{T}}_{\mathrm{R}}$ refers to the total retention times (chart distances) measured under the conditions of temperature programming. The value of I^{T} will usually differ from the value of I measured for the same compound under isothermal conditions, using the same two phases.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 844
Orange Book, p. 108

retention temperature

in chromatography

The column temperature when the peak maximum for a component has been reached in temperature-programmed chromatography.

Source:
Orange Book, p. 105

retention time

in chromatography

See: hold-up volume (time), relative retention, retention factor, retention index, retention volumes, total retention volume (time)

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 841

retention volumes

Also contains definition of: adjusted retention volume *in chromatography*

in chromatography

Retention measurements (and measurements of hold-up volume and peak width) may be made in terms of times or chart distances as well as volumes. If flow and recorder speeds are constant, the volumes are directly proportional to the times and chart distances. The following definitions are drawn up in terms of volume, and it is recommended that theoretical discussion should be couched in the same terms wherever possible. The total retention volume, V_{R}, is the volume of eluent carrier gas admitted to the column between the injection of the sample and the emergence of the peak maximum of the specified component. It includes the hold-up volume. In gas chromatography, the volume of carrier gas is specified at the outlet pressure and temperature of the column. Note: the word 'total' in this definition allows retention time to be used as a general term when specification of a particular quantity is not required. The adjusted retention volume, $V_{\mathrm{R}}^{'}$, is the total retention volume less the hold-up volume, V_{M}, i.e.

$$V_{\mathrm{R}}^{'} = V_{\mathrm{R}} - V_{\mathrm{M}} = \bar{V} - V_{\mathrm{I}}$$

where $\bar{V}$ is the peak elution volume and V_{I} the interstitial volume. The net retention volume, V_{N}, is the adjusted retention volume multiplied by the pressure-gradient correction factor:

$$V_{\mathrm{N}} = j\, V_{\mathrm{R}}^{'}$$

The specific retention volume, V_{g}, is the net retention volume per gram of stationary liquid, active solid or solvent-free gel. In liquid chromatography, except when conducted at very high pressures, the compression of the mobile phase is negligible, and the adjusted and net retention volumes are identical. The specific retention volume is then the adjusted retention volume per gram of stationary liquid, active solid, or solvent-free gel. It is recommended that, when appropriate, authors specify the drying conditions. At 0 °C,

$$V_g = 273 \frac{V_N}{w_L T}$$

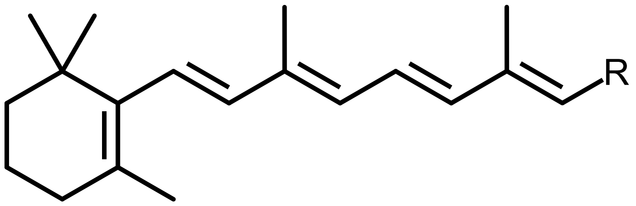
where w_L is the mass of the stationary liquid phase.

Source:
Orange Book, p. 103
Orange Book, p. 104

See also:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 841

retinoids

Oxygenated derivatives of 3,7-dimethyl-1-(2,6,6-trimethylcyclohex-1-enyl)nona-1,3,5,7-tetraene as shown and derivatives thereof.



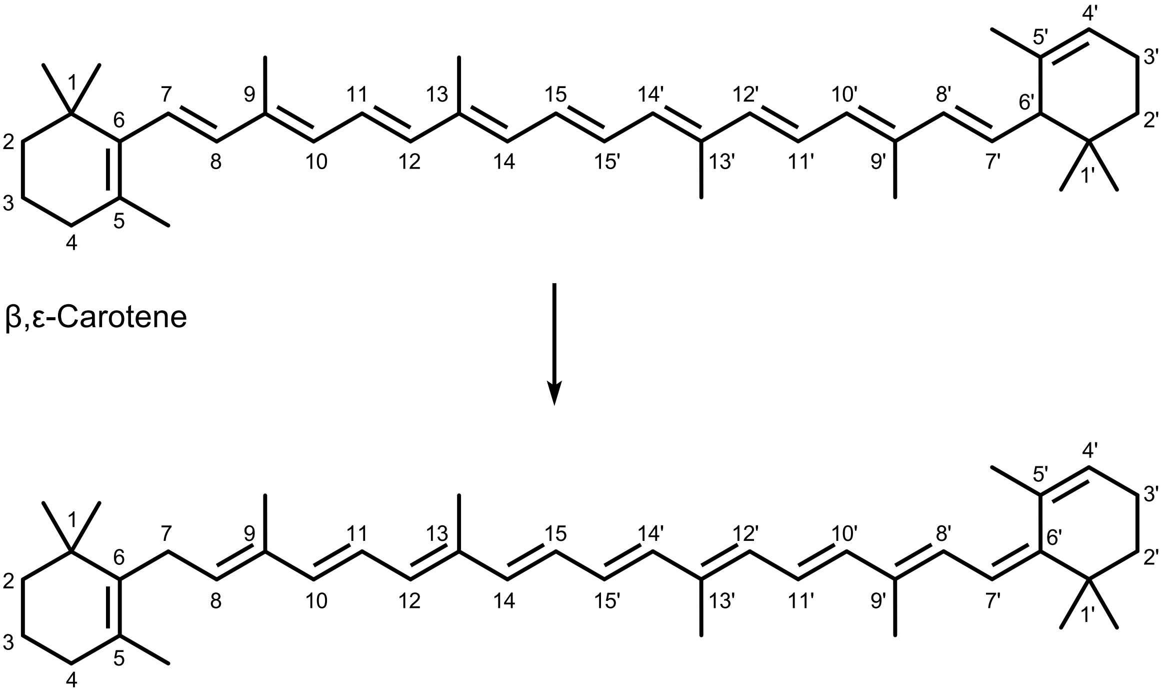
See also: carotenoids, retro

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1363

See also:
White Book, p. 247

retro

1. A prefix which indicates a shift by one position of all single and double bonds in a conjugated polyene system. It has been applied only to carotenoids and retinoids, e.g. *retro*-carotenoids, *retro*-retinoids.



β,ε-Carotene

6',7-*retro*-β,ε-Carotene

2. A prefix which indicates the reverse sequence of a peptide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1363
Blue Book (Guide), p. 32

See also:
White Book, p. 229
White Book, p. 249
White Book, p. 64

retroaddition [obsolete]

See: cycloelimination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1161

retrocycloaddition [obsolete]

See: cycloelimination

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1161

reverse osmosis

Liquid-phase pressure-driven separation process in which applied transmembrane pressure causes selective movement of solvent against its osmotic pressure difference.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1489

reverse transcriptases

Enzymes found in retroviruses that can synthesize complementary single-strands of DNA from an mRNA sequence as template They are used in genetic engineering to produce specific cDNA molecules from purified preparations of mRNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

reversed direct-injection burner

in analytical flame spectroscopy

A direct-injection burner combines the function of nebulizer and burner. Most commonly the oxidant is also used for aspirating and nebulizing the sample. However, when the fuel is used for this purpose, the term reversed direct-injection burner is applied.

Source:
Orange Book, p. 166

reversed (radiochemical) isotope dilution analysis

Isotope dilution analysis used for the determination of the isotopic carrier in a solution of a radionuclide with the aid of one of its stable isotopes.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

reversed-phase chromatography

An elution procedure used in liquid chromatography in which the mobile phase is significantly more polar then the stationary phase, e.g. a microporous silica-based material with chemically bonded alkyl chains. The term 'reverse phase' is an incorrect expression to be avoided.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 826
Orange Book, p. 93

reversible network

Polymer network that forms or breaks up as the temperature is changed or under the action of a force.
Note:
The junction points in a reversible network are usually small crystallites or glassy domains such as those formed within block copolymers.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1815

reversible transition

A transition that returns a system directly to its original state by reversing the process that changed it.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 589

revolutions per minute (rpm)

Non-SI unit for rotational frequency.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 991

$R_F$value

in chromatography

See: retardation factor *in planar chromatography*

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 845
Orange Book, p. 105

rheology

The study of the flow and deformation of matter under the influence of a mechanical force. It is concerned particularly with material behaviour which cannot be described by the simple linear models of hydrodynamics and elasticity. Some of these departures are due to the presence of colloidal particles or to the influence of surfaces.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1215

rheopexic gel

Also contains definition of: rheotropic gel

Gel for which the time of solidification after discontinuation of a relatively high shear rate, is reduced by applying a small shear rate.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1808

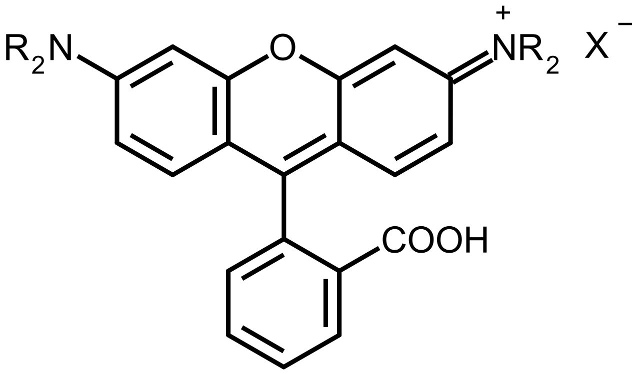
rheopexy

A phenomenon in which the time of solidification, after discontinuation of a relatively high shear rate, is shortened by applying a small shear rate.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

rhodamine dyes

Dyes derived from condensation of phthalic anhydride with *m*-dialkylaminophenols.



See: xanthene dyes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1363

rhombohedral graphite

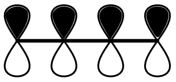
A thermodynamically unstable allotropic form of graphite with an ABCABC stacking sequence of the layers. The exact crystallographic description of this allotropic form is given by the space group $D^5_{3\,\mathrm{d}} - R\bar{3}m$, (unit cell constants: $a = 256.6\ \mathrm{pm}$, $c = 1006.2\ \mathrm{pm}$).
Note:

The structure of rhombohedral graphite can be best considered as an extended stacking fault in hexagonal graphite. Rhombohedral graphite can not be isolated in pure form (natural graphite and laboratory preparations contain less than 40% of rhombohedral graphite in combination with hexagonal graphite). It is produced by shear deformation of hexagonal graphite and transforms progressively to the hexagonal (ABAB) modification on heating above 1600 K.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 504

ribbon delocalisation

Electron delocalization realized in both acyclic and cyclic π-conjugated, **1**, and σ-bonded, **2**, ribbon-like systems.



1

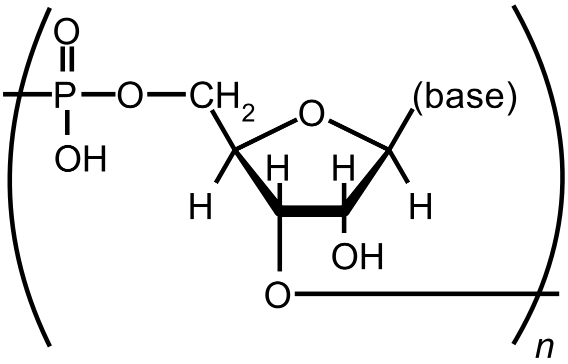
2

For cyclic systems, a variety of linkage fashions between several ribbons (pericyclic, spirocyclic, longicyclic and laticyclic) is possible.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1961

ribonucleic acids (RNA)

Naturally occurring polyribonucleotides.



See also: nucleic acids, nucleosides, nucleotides, ribonucleotides, messenger RNA, transfer RNA, ribosomal RNA

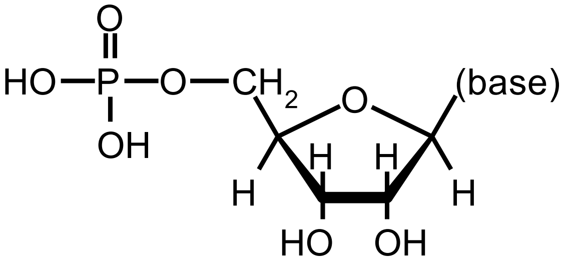
Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1364

See also:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

White Book, p. 110

ribonucleotides

Nucleotides in which the glycosyl group is a ribosyl group.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1364

See also:
White Book, p. 109

ribosomal RNA (rRNA)

RNA molecules which are essential structural and functional components of ribosomes, the subcellular units responsible for protein synthesis.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

ribosomes

Subcellular units composed of specific RNA molecules and a large number of proteins that are responsible for protein synthesis.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

Rice–Ramsperger–Kassel (RRK) theory

A theory of unimolecular gas reactions in which the rate with which the energized reactant molecule breaks down is treated as a function of the energy ε that it contains. The theory assumes that the rate is proportional to the number of ways of distributing ε among the internal degrees of freedom of the reactant molecule, in such a manner that the critical energy ε_{c} is localized in one particular degree of freedom.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 185

Rice–Ramsperger–Kassel–Marcus (RRKM) theory

An improved form of Rice–Ramsperger–Kassel (RRK) theory in which account is taken of the way in which the various normal-mode vibrations and rotations contribute to reaction, and allowance is made for the zero-point energies. In this theory the energy ε^* in an energized molecule is classified as either active, $\varepsilon^{*\text{active}}$, or inactive, $\varepsilon^{*\text{inactive}}$. The rate depends upon $\frac{P(\varepsilon^{*\text{active}})}{N(\varepsilon^*)}$, where $N(\varepsilon^*)$ is the density of states having energy between ε^* and $\varepsilon^* + \mathrm{d}\varepsilon^*$, and $P(\varepsilon^{*\text{active}})$ is the sum of the active quantum states of the activated complex. This extension of RRK theory brings it in line with transition-state theory.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 186

riffling

in analytical chemistry

The separation of a free-flowing sample into (usually) equal parts by means of a mechanical device composed of diverter chutes.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1204

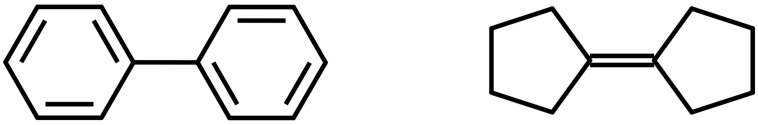
rigid chain

The rod-like chain of an MCPLC (main-chain polymer liquid crystal) with direct links between the mesogenic groups for which the persistence length is at least comparable with the contour length and much greater than the diameter.

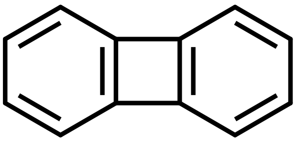
Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 505

ring assembly

Two or more cyclic systems (single rings or fused systems) which are directly joined to each other by double or single bonds are named ring assemblies when the number of such direct ring junctions is one less than the number of cyclic systems involved. Examples:



Ring assemblies



Fused polycyclic systems

Source:
Blue Book, p. 42

ring reversal (ring inversion)

The interconversion by rotation about single bonds (coupled with angle deformation in the transition state) of cyclic conformers having equivalent ring shapes (e.g. chair → chair) though not necessarily equivalent spatial positions of substituents (e.g. equatorial → axial).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2217

ring-opening copolymerization

A copolymerization which is a ring-opening polymerization with respect to at least one monomer.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2308

ring-opening polymerization

A polymerization in which a cyclic monomer yields a monomeric unit which is acyclic or contains fewer cycles than the monomer.
Note:
If the monomer is polycyclic, the opening of a single ring is sufficient to classify the reaction as ring-opening polymerization.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2308

ring-sector

Also contains definitions of: atomic ring-sector, bond ring-sector

A sequence of ring atoms, linked together as an unbranched chain and connecting two bridgeheads or junctions, but not itself containing any bridgehead or junction, is termed an atomic ring-sector. A bond linking together directly two bridgeheads or junctions is termed a bond ring-sector.

Source:
Blue Book, p. 499

Ringelmann chart

in atmospheric chemistry

A chart which has been used in air pollution evaluation for assigning the degree of blackness of smoke emanating from a source. The observer compares the shades of grey (white to black) with a series of shade diagrams formed by horizontal and vertical black grid lines on a white background. A corresponding number, the Ringelmann number, is then assigned to the describe the best match; numbers range from 0 (white) to 5 (black). This method of pollution evaluation, although relevant to the enforcement of legislation still in force in many countries, is not recommended for use today since more quantitative indicators of the efficiency of the combustion are now available.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2211

ringing gel

Also contains definition of: humming gel

Gel with energy dissipation in the acoustic frequency range.
Note:
A ringing gel is often a hydrogel with a surfactant as a third component and has a composition within an isotropic, one-phase region of its ternary phase diagram.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1808

rise time

of an analyser

The difference between the response time and the dead time.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

risk

1. Probability of adverse effects caused under specified circumstances by an agent in an organism, a population, or an ecological system.
2. Expected frequency of occurrence of a harmful event arising from such an exposure.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1069

risk assessment

Identification and quantification of the risk resulting from a specific use or occurrence of an agent, taking into account possible harmful effects on individuals exposed to the agent in the amount and manner proposed and all the possible routes of exposure.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1069

risk estimation

Assessment with or without mathematical modeling, of the probability and nature of effects of exposure to a substance based on quantification of dose-effect and dose-response relationships for that substance and the population(s) and environmental components likely to be exposed and on assessment of the levels of potential exposure of people, organisms, and environment at risk.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1023

Ritchie equation

The linear free-energy relation

$$\log_{10} k_{\mathrm{N}} = \log_{10} k_0 + N_+$$

applied to the reactions between nucleophiles and certain large and relatively stable organic cations, e.g. arenediazonium, triarylmethyl and aryltropylium cations in various solvents. k_{N} is the rate constant for reaction of a given cation with a given nucleophilic system (i.e. given nucleophile in a given solvent). k_0 is the rate constant for the same cation with water in water, and N_+ is a parameter which is characteristic of the nucleophilic system and independent of the cation. A surprising feature of the equation is the absence of a coefficient of N_+, characteristic of the substrate (*cf.* the s in the Swain–Scott equation), even though values of N_+ vary over 13 log units. The equation thus involves a gigantic breakdown of the reactivity–selectivity principle. The equation has been extended both in form and in range of application.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1161

R_M value

in planar chromatography

A logarithmic function of the R_F value (retardation factor):

$$R_\mathrm{M} = \log_{10}\left(\frac{1 - R_\mathrm{F}}{R_\mathrm{F}}\right) = \log_{10}\left(\frac{1}{R_\mathrm{F}} - 1\right)$$

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 845

rod-like morphology

Morphology characterized by cylindrical phase domains.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2004

röntgen

Non-SI unit of exposure to X- or γ-radiation: $\mathrm{R} = 2.58 \times 10^{-4}\ \mathrm{C\ kg}$.

Source:
Green Book, 2nd ed., p. 113
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 991

root-mean-square end-to-end distance, $< r^2 >^{1/2}$

in polymers

The square root of the mean-square end-to-end distance of a linear polymer chain averaged over all conformations of the chain. For a freely jointed chain consisting of N segments each of length L, it is given by:

$$< r^2 >^{1/2} = \sqrt{N}\ L$$

The subscript zero is used to indicate unperturbed dimensions, as in $< r^2 >_0^{1/2}$. If this term is used repeatedly, and if it is not confusing, the abbreviated name 'end-to-end distance' may be used.

Source:
Purple Book, p. 49

rotamer

One of a set of conformers arising from restricted rotation about one single bond.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2217

rotational barrier

In a rotation of groups about a bond, the potential energy barrier between two adjacent minima of the molecular entity as a function of the torsion angle.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2217

rotational constants

Coefficients of quantum numbers in the rotational term expression and inversely proportional to the principal moments of inertia. Symbols: A, B, C. $\widetilde{A} = \frac{h}{8\,\pi^2\,c\,I_{\mathrm{A}}}$ (dimension wavenumber), $A = \frac{h}{8\,\pi^2\,I_{\mathrm{A}}}$ (dimension frequency) where h is the Planck constant and c the speed of light in vacuum.

Source:
Green Book, 2nd ed., p. 23

rotational correlation time, τ_{c} or θ

Parameter describing the time dependence of the tumbling of a molecular entity in a medium of viscosity η. The rotational correlation time can be obtained from the decay of the fluorescence or phosphorescence anisotropy and is related to the average molecular rotational diffusion coefficient, D_{r}, in turn related to the hydrodynamic molecular volume of the fluorophore, V, and to η (see Note 3).
Notes:

1. Mathematical definition: $r(t) = r_0 \exp(-\frac{t}{\tau_{\mathrm{c}}})$ with $r(t)$ the emission anisotropy at time t and r_0 the fundamental emission anisotropy.
2. In the case of a spherical emitting species reorienting itself in a homogeneous fluid, $\tau_{\mathrm{c}} = \frac{1}{6\,D_{\mathrm{r}}}$.
3. Often, the Stokes–Einstein relationship is used for the calculation of D_{r}, i.e., $D_{\mathrm{r}} = R\,T\,/\,6\,V\,\eta$ with R the gas constant, T the absolute temperature and V the hydrodynamic molecular volume. However, the use of this relationship at a molecular level is questionable, and D_{r} should be independently determined by time-resolved fluorescence polarization methods. Compare with rotational relaxation time.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 416

rotational diffusion

A process by which the equilibrium statistical distribution of the overall orientation of molecules or particles is maintained or restored. Rotational diffusion may be compared to translational diffusion through which the equilibrium statistical distribution of position in space is maintained or restored.

Source:
Purple Book, p. 61

rotational diffusion coefficient

Defined by the equation:

$$D_\theta = \frac{t_\theta}{\frac{\partial(f(\theta,\,\Phi))}{\partial\theta}\sin\theta}$$

where $f(\theta,\,\Phi)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\Phi$ is the fraction of particles whose axes make an angle between θ and $\theta+\mathrm{d}\theta$ with the direction $\theta=0$, and have an azimuth between Φ and $\Phi+\mathrm{d}\Phi$; $t_\theta\,\mathrm{d}\Phi$ is the fraction of particles having an azimuth between Φ and $\Phi+\mathrm{d}\Phi$ whose axis passes from values $<\theta$ to values $>\theta$ in unit time. The axis whose rotational diffusion is considered has to be clearly indicated.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 617

rotational frequency, f_{rot}

in centrifugation

The number of rotations divided by time:

$$f_{\mathrm{rot}} = \frac{\mathrm{d}N}{\mathrm{d}t}$$

The synonyms rate of rotation, rate of revolution, centrifugal speed, centrifugation speed, and the traditional units of rotational frequency such as revolutions per minute, r.p.m., ppm, $\mathrm{rev.\ min}^{-1}$, $\mathrm{r\ min}^{-1}$, are not recommended.

Source:
PAC, 1994, *66*, 897 *(Quantities and units for centrifugation in the clinical laboratory (IUPAC Recommendations 1994))* on page 904
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 991

rotational relaxation time, ρ

Parameter describing the time-dependence of the tumbling of a molecular entity in a medium of viscosity η as originally defined by Debye, and used by Perrin in the original development of the theories of rotational motion of fluorophores.
Note:
Related to the rotational correlation time, τ_c, by $\rho = 3\ \tau_c$. Thus, in the case of a spherically emitting species reorienting itself in a homogeneous fluid, $\rho = 1/(6\ D_r)$, with D_r the rotational diffusion coefficient.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 416

rotational term, *F*

Rotational energy divided by the product of the Planck constant and the speed of light.
See: term

Source:
Green Book, 2nd ed., p. 23

rotator phase transition

A transition from a fully-ordered crystal of globular or quasi-spherical molecules to a crystal that retains translational order but exhibits dynamic orientational disorder and is usually mechanically soft (plastic phase). Example: The transition of CBr_4 to a plastic phase which exists from 319 to 365 K.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 589

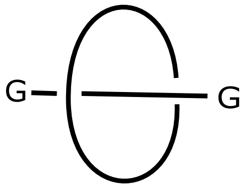
rotatory power

The quantitative measure of optical activity.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2217

rotaxanes

Molecules in which a ring encloses another, rod-like molecule having end groups too large to pass through the ring opening, and thus holds the rod-like molecule in position without covalent bonding.

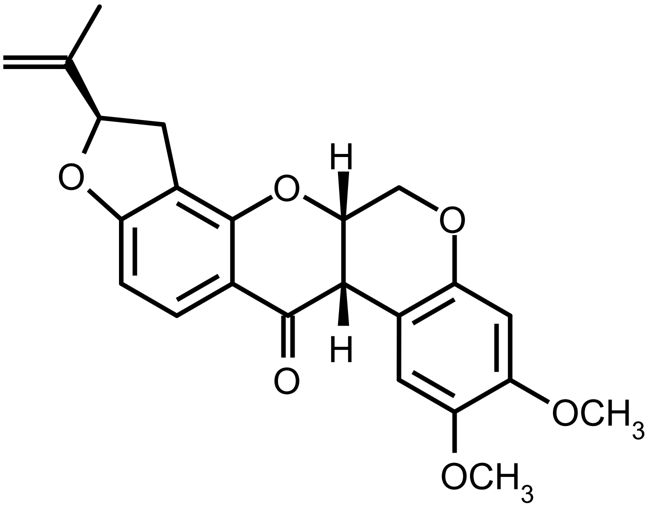


See: catenanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1364

rotenoids

Naturally occurring substances containing a *cis*-fused tetrahydrochromeno[3,4-*b*]chromene nucleus. Many rotenoids contain an additional ring, e.g rotenone:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1364

rotometer

in atmospheric chemistry

A device, based on Stokes law, for measuring rate of fluid flow. It is a tapered vertical tube having a circular cross-section in which a float moves in a vertical path to a height dependent upon the rate of fluid flow upward through the tube.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2211

roughness factor (rugosity)

of a surface

The ratio:

$$f_r = \frac{A_r}{A_g}$$

where A_r is the real (true, actual) surface (interface) area and A_g is the geometric surface (interface) area.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 439

rovibronic state

A state corresponding to a particular rotational sublevel of a particular vibrational level of a particular electronic state.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2271

rubredoxin

An iron-sulfur protein without acid-labile sulfur, in which an iron centre is coordinated by four sulfur-containing ligands, usually cysteine. The function, where known, is an electron carrier.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1296

ruby laser

A pulsed source of coherent radiation emitting mainly at 694.3 nm from chromium ions (Cr^{3+}) in aluminium oxide.
See: laser, solid state lasers

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2272

rupture

of a thin film

The formation of a hole which permits coalescence or direct contact of the two phases which it separates.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

Rutherford backscattering (RBS)

Synonym: backscattering spectroscopy

Any technique using high energy particles directed toward a sample, in which the bombarding particles are detected and recorded as function of energy and/or angle. The technique is mostly used for determining depth distributions of elements based on the energy of the backscattered particle. In general, He^+ or H^+ particles are used at energies in the order of $100\ \mathrm{keV}$ to some MeV. Also referred to as backscattering spectrometry (BSS).

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2246

Rydberg constant

Atomic fundamental physical constant $R_{\infty} = \frac{E_h}{2\,h\,c_0} = 1.097\ 373\ 1534\ (13) \times 10^7\ \mathrm{m}^{-1}$, where E_h is the Hartree energy, h the Planck constant, and c_0 the speed of light.

Source:
CODATA Bull. 1986, *63*, 1

Rydberg orbital

For an atom, an orbital with principal quantum number greater than that of any occupied orbital of the ground state. For a molecular entity, a molecular orbital which correlates with a Rydberg atomic orbital in an atomic fragment produced by dissociation. Typically, the extension of the Rydberg orbital is large compared to the size of the atom or molecular entity.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2272

Rydberg state

An electronic state that arises by the excitation of a valence electron to a diffuse atomic-like orbital. For instance, the lowest lying Rydberg state (n, 3S) of NH_3 can be described as resulting from the excitation of a non-bonding orbital to a 3S Rydberg orbital.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1961

Rydberg transition

An electronic transition described approximately as promotion of an electron from a 'bonding' orbital to a Rydberg orbital. Spectral bands corresponding to Rydberg transitions approximately fit the Rydberg formula:

$$\sigma = I - \frac{R}{(n - \Delta)^2}$$

where σ is the wavenumber, I the ionization potential of the atom or molecular entity, n a principal quantum number, R the Rydberg constant, and Δ the quantum defect which differentiates between s, p, d, etc., orbitals. The notation used is, e.g. $\pi \rightarrow \mathrm{ns}$.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2272

σ, π (sigma, pi)

The terms are symmetry designations, π molecular orbitals being antisymmetric with respect to a defining plane containing at least one atom (e.g. the molecular plane of ethene) and σ molecular orbitals symmetric with respect to the same plane. In practice the terms are used both in this rigorous sense (for orbitals encompassing the entire molecule) and also for localized two-centre orbitals or bonds, and it is necessary to make a clear distinction between the two usages. In the case of two-centre bonds, a π-bond has a nodal plane that includes the internuclear bond axis, whereas a σ-bond has no such nodal plane. (A δ-bond in organometallic or inorganic molecular species has two nodes.) Radicals are classified by analogy into σ- and π-radicals. Such two-centre orbitals may take part in molecular orbitals of σ- or π-symmetry. For example, the methyl group in propene contains three C–H bonds, each of which is of local σ-symmetry (i.e. without a nodal plane including the internuclear axis), but these three 'σ-bonds' can in turn be combined to form a set of group orbitals one of which has π-symmetry with respect to the principal molecular plane and can accordingly interact with the two-centre orbital of π-symmetry (π-bond) of the double-bonded carbon atoms, to form a molecular orbital of π-symmetry. Such an interaction between the CH_3 group and the double bond is an example of what is called hyperconjugation. This cannot rigorously be described as 'σ–π conjugation' since σ and π here refer to different defining planes, and interaction between orbitals of different symmetries (with respect to the same defining plane) is forbidden.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1163

σ → σ* transition

An electronic transition described approximately as promotion of an electron from a 'bonding' σ orbital to an 'antibonding' σ orbital designated as σ^*. Such transitions generally involve high transition energies, and appear close to or mixed with Rydberg transitions.

Source:
PAC, 1996, *68*, 2223 ***(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))*** on page 2279

σ-adduct

The product formed by the attachment of an electrophilic or nucleophilic entering group or of a radical to a ring carbon of an aromatic species so that a new σ-bond is formed and the original conjugation is disrupted. (This has generally been called a 'σ-complex', but adduct is more appropriate than complex according to the definitions given.) The term may also be used for analogous adducts to unsaturated (and conjugated) systems in general.
See also: Meisenheimer adduct

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1170

σ-bond

See: σ, π

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1171

σ-constant

Specifically the substituent constant for *meta*- and for *para*-substituents in benzene derivatives as defined by Hammett on the basis of the ionization constant of a substituted benzoic acid in water at 25 °C, i.e. $\log_{10}\left(\frac{K_{\mathrm{a}}}{K_{\mathrm{a}}^{0}}\right)$), where K_{a} is the ionization constant of a *m*- or *p*-substituted benzoic acid and K_{a}^{0} that of benzoic acid itself. The term is also used as a collective description for related electronic substituent constants based on other standard reaction series, of which, σ^{+}, σ^{-} and σ^{0} are typical; also constants which represent dissected electronic effects such as σ_{I} and σ_{R}. For this purpose it might be better always to spell out the term in full, i.e. as 'Hammett sigma constant', and restrict σ-constants to the scale of substituent constants which is based on benzoic acid. A large positive σ-value implies high electron-withdrawing power by inductive and/or resonance effect, relative to H; a large negative σ-value implies high electron-releasing power relative to H.
See also: Hammett equation, ρ-value, Taft equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1171

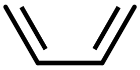
σ-orbital

See: σ, π

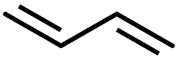
Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1171

s-*cis*, s-*trans*

The spatial arrangement of two conjugated double bonds about the intervening single bond is described as s-*cis* if synperiplanar and s-*trans* if antiperiplanar. This term should not be applied to other systems such as *N*-alkyl amides (use *E/Z* or *sp/ap*).



s-*cis*



s-*trans*

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2217

saccharides

The monosaccharides and di-, oligo - and polysaccharides, which are made up of *n* monosaccharide units linked to each other by a glycosidic bond. Considered by some to be synonymous with carbohydrates.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1364

Sackur–Tetrode constant

Fundamental physical constant representing the translational contribution to molar entropy; $\frac{S_0}{R} = -1.151\,693(21)$ at 1 K and standard pressure of 100 kPa, where R is the gas constant.

Source:
CODATA Bull. 1986, *63*, 1

sacrificial acceptor

Molecular entity that acts as the electron acceptor in a photoinduced electron transfer process and is not restored in a subsequent oxidation process but is destroyed by irreversible chemical conversion.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2272

sacrificial donor

Molecular entity that acts as the electron donor in a photoinduced electron transfer process and is not restored in a subsequent reduction process but is destroyed by irreversible chemical conversion.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2272

salt

A chemical compound consisting of an assembly of cations and anions.

Source:
Red Book, p. 118

salt effect [obsolete]

See: kinetic electrolyte effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

salt form of an ion exchanger

The ionic form of an ion exchanger in which the counter-ions are neither hydrogen nor hydroxide ions. When only one valence is possible for the counter-ion, or its exact form or charge is not known, the symbol or the name of the counter-ion without charge is used, e.g. sodium-form or Na-form, tetramethylammonium-form, orthophosphate-form. When one of two or more possible forms is exclusively present, the oxidation state may be indicated by a Roman numeral, e.g. Fe^{II} form, Fe^{III} form.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 855

salting out

The addition of particular electrolytes to an aqueous phase in order to increase the distribution ratio of a particular solute.
Notes:

1. The addition of electrolytes to improve phase separation behaviour should not be referred to as salting out.
2. The term is also used for the addition of electrolytes to reduce the mutual partial miscibility of two liquids.
3. It has no connection with synergism.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2379

sample error

in spectrochemical analysis

An error which arises when the absorbance of some samples changes with time, e.g. as a result of photochemical reaction, formation of aggregates or adsorption on the cell wall.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1457

sample handling

in analysis

Any action applied to the sample before the analytical procedure. Such actions include the addition of preservatives, separation procedures, storage at low temperature, protection against light and irradiation, loading, etc.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

sample

in analytical chemistry

A portion of material selected from a larger quantity of material. The term needs to be qualified, e.g. bulk sample, representative sample, primary sample, bulked sample, test sample. The term 'sample' implies the existence of a sampling error, i.e. the results obtained on the portions taken are only estimates of the concentration of a constituent or the quantity of a property present in the parent material. If there is no or negligible sampling error, the portion removed is a test portion, aliquot or specimen. The term 'specimen' is used to denote a portion taken under conditions such that the sampling variability cannot be assessed (usually because the population is changing), and is assumed, for convenience, to be zero. The manner of selection of the sample should be prescribed in a sampling plan.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1200

PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

See also:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1465

sample injector

in chromatography

A device by which a liquid or gaseous sample is introduced into the apparatus. The sample can be introduced directly into the carrier-gas stream, or into a chamber temporarily isolated from the system by values which can be changed so as to make an instantaneous switch of the gas stream through the chamber. The latter is a by-pass injector.

Source:
Orange Book, p. 98

sample unit

The discrete identifiable portion suitable for taking as a sample or as a portion of a sample. These units may be different at different stages of sampling.

Source:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1463

sampler

A device used to withdraw and deliver a volume or an amount of a sample.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

sampling error

That part of the total error (the estimate from a sample minus the population value) associated with using only a fraction of the population and extrapolating to the whole, as distinct from analytical or test error. It arises from a lack of homogeneity in the parent population. In chemical analysis, the final test result reflects the value only as it exists in the test portion. It is usually assumed that no sampling error is introduced in preparing the test sample from the laboratory sample. Therefore, the sampling error is usually associated exclusively with the variability of the laboratory sample. Sampling error is determined by replication of the laboratory samples and their multiple analyses. Since sampling error is always associated with analytical error, it must be isolated by the statistical procedure of analysis of variance.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1201

sampling interval

in electroanalysis

In Tast polarography, square-wave polarography, and similar techniques, the interval during which the current is measured or recorded.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1504

sampling plan

in analytical chemistry

A predetermined procedure for the selection, withdrawal, preservation, transportation and preparation of the portions to be removed from a population as samples. Summarizing the test values or observations from the selected portions yields an estimate for the concentration of an analyte or a value for a property determined with a calculable degree of uncertainty at a specified confidence level. A sampling plan includes the designation of the number, location and size of the portions, and instructions for the extent of compositing and for the reduction (in amount and fineness) of the portions to a laboratory sample and to test portions. It may also contain acceptance criteria. Some sampling plans do not include more than instructions for the statistical selection of portions to be removed. Such plans should properly be designated as 'statistical sampling plans'.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1201

sampling time

in electroanalysis

In Tast polarography, square-wave polarography, and similar techniques, the duration of the sampling interval.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1504

sandwich compounds

Compounds in which a metal atom is located between the faces of two parallel and planar (or nearly so) ring structures, e.g. bis(η^5-cyclopentadienyl)iron (ferrocene), dibenzenechromium.
See also: metallocenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1364

sanitary land fill

An engineered burial of refuse. The refuse is dumped into trenches and compacted by bulldozer, where, it is hoped, aerobic metabolism by microorganisms decomposes the organic matter to stable compounds (H_2O, CO_2, etc.). Moisture is essential for the biological degradation and groundwater assists the process except when it fills air voids and prevents the transport of oxygen to the refuse. Land fills of unsatisfactory design can be major sources of air, water and soil pollution.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2212

saprophyte

A microorganism that feeds on dead and decaying organic matter. Saprophytes excrete enzymes that digest organic residues externally, the low molecular weight compounds formed then being absorbed.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

saturated solution

A solution which has the same concentration of a solute as one that is in equilibrium with undissolved solute at specified values of the temperature and pressure.

Source:
Orange Book, p. 83

saturation

The state of a saturated solution.

Source:
Orange Book, p. 18

saturation activity

For a specified isotope, the value of the activity of an irradiated element, whence state of saturation is reached.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

saturation fraction, s_B

Amount-of-substance of a component (solute) in a solution divided by the amount-of-substance of the component when it is saturating the system at constant temperature and pressure. Also referred to simply as saturation, for example oxygen saturation.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 991

saturation

in radioanalytical chemistry

Of an irradiated element for a specified isotope, the steady state reached when the disintegration rate of the nuclide formed is equal to its production rate.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

saturation transfer

A term used in nuclear magnetic resonance. When a nucleus is strongly irradiated, its spin population may partly be transferred to another nucleus by an exchange process.
See: magnetization transfer

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

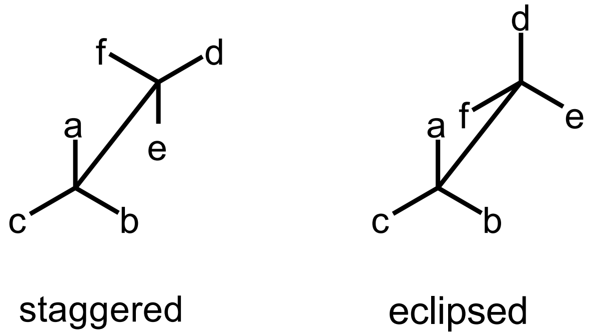
saturation vapour pressure

The pressure exerted by a pure substance (at a given temperature) in a system containing only the vapour and condensed phase (liquid or solid) of the substance.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2212

sawhorse projection

A perspective formula indicating the spatial arrangement of bonds on two adjacent carbon atoms. The bond between the two atoms is represented by a diagonal line, the left-hand bottom end of which locates the atom nearer the observer and the right-hand top end the atom that is further away. In general a Newman or zig-zag projection is preferred.



Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2217

Saytzeff rule

Synonym: Zaitsev rule

Dehydrohalogenation of secondary- and tertiary-alkyl halides proceeds by the preferential removal of the β-hydrogen from the carbon that has the smallest number of hydrogens. Originally formulated by A. Saytzeff (Zaitsev) to generalize the orientation in β-elimination *reactions* of alkyl halides, this rule has been extended and modified, as follows: When two or more olefins can be produced in an elimination reaction, the thermodynamically most stable alkene will predominate. Exceptions to the Saytzeff rule are exemplified by the Hofmann rule.
See also: Markownikoff rule

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

sc

See: torsion angle

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

scaler

A sub-assembly for counting electrical pulses and containing one or more scaling circuits.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1551

scaling circuit

An electronic circuit which produces an output pulse for each time a specified number of pulses has been received at its input.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1551

scaling factor

A variational parameter used as a multiplier of each nuclear Cartesian and electronic coordinate chosen to minimize the variational integral and to make a trial variation function to satisfy the virial theorem. In practical calculations, the numeral factor to scale computed values, e.g. vibrational frequencies, to those found in experiments.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1961

scanning electron microscopy (SEM)

Any analytical technique which involves the generation and evaluation of secondary electrons (and to a lesser extent back scattered electrons) by a finely focused electron beam (typically $10\ \mathrm{nm}$ or less) for high resolution and high depth of field imaging.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2024

scanning method

in mass spectrometry

This term refers to the sequence of control over operating parameters of a mass spectrometer that results in a spectrum of masses, velocities, momenta or energies.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2212

scanning transmission electron microscopy (STEM)

A special TEM-technique in which an electron transparent sample is bombarded with a finely focused electron beam (typically of a diameter of less than 10 nm) which can be scanned across the specimen or rocked across the optical axis and transmitted, secondary, back scattered and diffracted electrons as well as the characteristic X-ray spectrum can be observed. STEM essentially provides high resolution imaging of the inner microstructure and the surface of a thin sample (or small particles), as well as the possibility of chemical and structural characterization of micrometer and sub-micrometer domains through evaluation of the X-ray spectra and the electron diffraction pattern.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2025

scattering

A process in which a change in direction or energy of an incident radiation is caused by interaction with a *particle*, a system of particles, or a photon.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1551
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2212

scattering angle, θ

Synonym: angle of observation

The angle between the forward direction of the incident beam and a straight line connecting the scattering point and the detector. Synonymous with angle of observation.

Source:
Purple Book, p. 65
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2212

scattering cross-section, σ_{scat}

The scattering coefficient per particle ($\frac{\text{cm}^2}{\text{particle}}$);

$$b_{\text{scat}} = n\,\sigma_{\text{scat}}$$

where n is the number concentration of particles (particles cm^{-3}) and σ_{scat} is the scattering cross-section. b_{scat}, the scattering component of extinction due to gas and particles, is measured in the atmosphere using a nephelometer. For a homogeneous atmosphere it is related in theory to the meteorological range (L_{V}): $L_{\text{V}} = \frac{3.9}{b_{\text{scat}}}$; b_{scat} and b_{abs} represent the scattering and absorption coefficients per unit length for a light beam (of path length L) which has a spectral radiance (intensity) I_0 incident on a sample of air and I is the transmitted spectral radiance (intensity), $\ln\left(\frac{I_0}{I}\right) = L\,(b_{\text{scat}} + b_{\text{abs}})$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2212

scattering error

in spectrochemical analysis

The presence of particulate matter, emulsions, micelles, etc. may cause radiation scattering which will result in further attenuation of the transmitted beam and the measured absorbance will be too high. This error is called the *scattering error.*

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1457

scattering matrix

The Stokes parameters of scattered light are given by the matrix equation

$$\left(s_0,\, s_1,\, s_2,\, s_3\right) = \boldsymbol{F}\left(s_0^0,\, s_1^0,\, s_2^0,\, s_3^0\right)$$

where the 4, 4 scattering matrix $\boldsymbol{F}$ is comprised of 16 scattering matrix elements. These matrix elements, which may originate in theory or experiment, provide a complete description of the scattered radiation in terms of the incident radiation.

Source:
PAC, 1983, *55*, 931 *(Definitions, terminology and symbols in colloid and surface chemistry. Part 1.14: Light scattering (Provisional))* on page 934

scattering plane

The plane containing the incident light beam and the line from the centre of the scattering system to the observer.

Source:
PAC, 1983, *55*, 931 *(Definitions, terminology and symbols in colloid and surface chemistry. Part 1.14: Light scattering (Provisional))* on page 932

scattering vector

The vector difference between the wave propagation vectors of the incident and the scattered beam, both of length $\frac{2\pi}{\lambda}$, where λ is the wavelength of the scattered radiation in the medium.

Source:
Purple Book, p. 65

scavenger

A substance that reacts with (or otherwise removes) a trace component (as in the scavenging of trace metal ions) or traps a reactive reaction intermediate.
See also: inhibition

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

scavenging

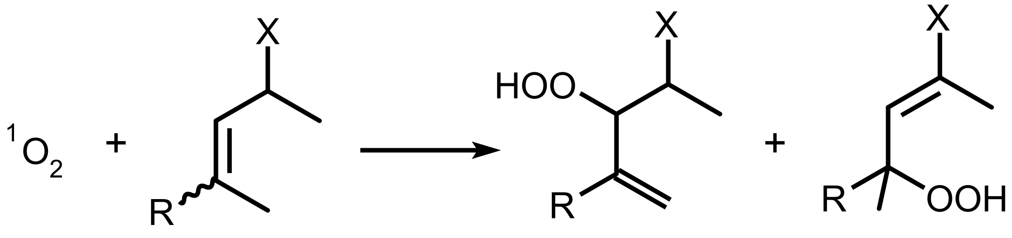
1. (*in radiation chemistry*) Binding radicals or free electrons with a receptive (or reactive) material.
2. (*in radiochemistry*) The use of a precipitate to remove from solution by absorption or coprecipitation, a large fraction of one or more radionuclides.

   Source:
   PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525
3. (*in atmospheric chemistry*) The removal of pollutants from the atmosphere by natural processes, including scavenging by cloud water, rainout and washout. This type of removal process is termed *precipitation scavenging*. Scavenging of airborne pollutants at the surfaces of plant, soil, etc., is termed *dry deposition*.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2213

Schenck reaction

The diastereoselective ene reaction of singlet molecular dioxygen with alkenes.
An example is:



Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 418

Schenck-sensitization mechanism

Chemical transformation of one molecular entity caused by photoexcitation of a sensitizer, which undergoes temporary covalent bond formation with the molecular entity (M).

$$\mathrm{S} + h\nu \longrightarrow {}^{*}\mathrm{S}$$

$$\mathrm{S} + \mathrm{M} \longrightarrow [{}^{*}\mathrm{S}\cdots\mathrm{M}]$$

Notes:

1. This mechanism is the basis of the Type I photooxygenation.
2. The reactive molecular entity could be ground-state molecular dioxygen, O_2, in which case energy transfer may occur producing singlet molecular oxygen, this being the basis of the Type II photooxygenation.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 418

Schiff bases (Schiff's bases)

Imines bearing a hydrocarbyl group on the nitrogen atom $R_2C{=}NR'$ ($R' \neq H$). Considered by many to be synonymous with azomethines.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1364

Schiller layers

Synonym: iridescent layers

In some systems, sedimenting particles form layers separated by approximately equal distances of the order of the wavelength of light. This gives rise to strong colours when observed in reflected light and the system is said to form iridescent layers or Schiller layers.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 611

Schulze–Hardy rule

The generalization that the critical coagulation concentration for a typical lyophobic sol is extremely sensitive to the valence of the counter-ions (high valence gives a low critical coagulation concentration).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

Schulz–Zimm distribution

In an assembly of macromolecules, a continuous distribution with the differential mass-distribution function of the form:

$$f_{\mathrm{w}}(x)\,\mathrm{d}x = \frac{a^{b}+1}{\Gamma(b+1)}\,x^{b}\,\mathrm{e}^{-a\,x}\,\mathrm{d}x$$

where x is a parameter characterizing the chain length, such as relative molecular mass or degree of polymerization, a and b are positive adjustable parameters, and ($\Gamma(b+1)$) is the gamma function of $(b+1)$.

Source:
Purple Book, p. 56

scintillation

Burst of luminescence of short duration caused by an individual energetic particle.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

scintillation counter

A scintillator coupled to a photomultiplier tube. Incident X-ray photons are converted in the scintillator into bursts of visible light photons, some of which fall on the photocathode and can be measured. For incident photons having energies higher than the absorption edge of the elements contained in the scintillator, an escape peak can be observed.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1753

scintillation detector

A radiation detector using a medium in which a burst of luminescence radiation, produced along the path of an ionizing particle, is quantified.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

scintillation spectrometer

A measuring assembly incorporating a scintillation detector and a pulse amplitude analyser used for determining the energy *spectrum* of certain types of radiation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1551

scintillators

Materials used for the measurement of radioactivity, by recording the radioluminescence. They contain compounds (chromophores) which combine a high fluorescence quantum efficiency, a short fluorescence lifetime, and a high solubility. These compounds are employed as solutes in aromatic liquids and polymers to form organic liquid and plastic scintillators, respectively.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2272
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

scrambling

See: isotopic scrambling

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

scrubber

in atmospheric chemistry

An apparatus used in sampling and in flue gas cleaning. The gas is passed through a space containing wetted 'packing' or spray. In general, particles are collected in scrubbers by one or a combination of the following: impingement of particles on a liquid medium; diffusion of the particles onto a liquid medium; condensation of liquid medium vapours on the particles; partitioning of the gas into extremely small elements to allow collection of the particles by Brownian diffusion and gravitation settling on the gas-liquid interface. The devices include spray towers, jet scrubbers, Venturi scrubbers, cyclonic scrubbers, inertial scrubbers, mechanical scrubbers and packed scrubbers. Normally the gas flow in the scrubber is counter to the liquid flow. Efficient scrubbers will collect particles as small as 1 to 2 μm in diameter.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2213

scrubbing

1. (*in solvent extraction*) : The process of selectively removing contaminating solutes (impurities) from an extract that contains these as well as the main extractable solute by treatment with a new immiscible liquid phase. The term stripping has a different meaning and should not be used in this sense although this usage has been customary in certain industries.

See also: crowding, stripping

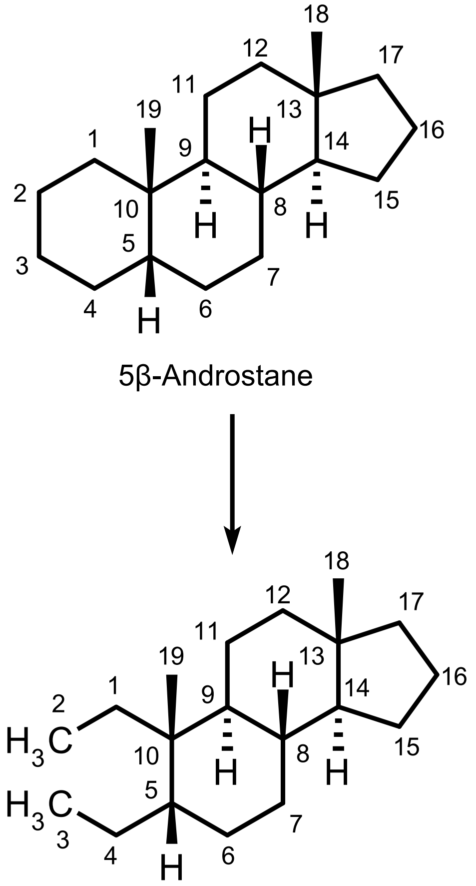
Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2388

2. (*in atmospheric chemistry*) : A process used in gas sampling or gas cleaning in which components in the gas stream are removed by contact with a liquid surface or a wetted packing, on spray drops, droplets, or in a bubbler, etc.

   Source:
   PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2213

seco-

Cleavage of a ring with addition of one or more hydrogen atoms at each terminal group thus created is indicated by the prefix 'seco'. Examples:



5β-Androstane

2,3-Seco-5β-androstane

Source:
Blue Book (Guide), p. 31

second

SI base unit of time (symbol: s). The second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium-133 atom.

Source:
Green Book, 2nd ed., p. 70
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 991

second messenger

Intracellular effector substance increasing or decreasing as a response to the stimulation of a receptor by an agonist, considered as the 'first messenger'.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1070

second

of arc

Non-SI unit of plane angle: $1'' = \frac{1}{3600}{}^\circ = 4.848\ 137 ... \times 10^{-6}\ \mathrm{rad}$.

Source:
Green Book, 2nd ed., p. 113
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 991

second-order transition

Synonym: continuous transition

A transition in which a crystal structure undergoes a continuous change and in which the first derivatives of the Gibbs energies (or chemical potentials) are continuous but the second derivatives with respect to temperature and pressure (i.e. heat capacity, thermal expansion, compressibility) are discontinuous. Example: The order-disorder transition in metal alloys, for example, CuZn. Synonymous with continuous transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 589

secondary crystallization

Crystallization occurring after primary crystallization, usually proceeding at a lower rate.

Source:
Purple Book, p. 85

secondary electron multiplier

in mass spectrometry

A device to multiply current in an electron beam (or in a photon or particle beam by first conversion to electrons) by incidence of accelerated electrons upon the surface of an electrode which yields a number of secondary electrons greater than the number of incident electrons. These electrons are then accelerated to another electrode (or another part of the same electrode), which in turn emits further secondary electrons so that the process can be repeated. It is recommended that one should refer to the abundance of an ion, to the intensity of an ion beam, and to the height or area of a peak.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1554
Orange Book, p. 204

secondary electron yield

in in situ microanalysis

The number of secondary electrons generated per primary electron for a given specimen and experimental conditions. It depends on the (mean) atomic number of the excited area of the sample, the angle between electron beam and sample surface, the primary electron energy, thickness of the sample and sample potentials.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2026

secondary electrons (se)

in in situ microanalysis

All electrons emitted from the surface of a solid except back scattered primary electrons. In practice, electrons emitted from the surface of a solid under particle bombardment which have a kinetic energy of less than $50\ \mathrm{eV}$.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2026

secondary fluorescence

in X-ray emission spectroscopy

Ionization of the analyte element in a sample by characteristic radiation from other elements in the sample resulting in an enhancement of the signal measured.

Source:
PAC, 1980, *52*, 2541 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - IV X-ray emission spectroscopy)* on page 2547

secondary ionization

in mass spectrometry

The process in which ions are ejected from a sample surface (which may be a solid or substrate dissolved in a solvent matrix) as a result of bombardment by a primary beam of atoms or ions.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548

secondary isotope effect

A kinetic isotope effect that is attributable to isotopic substitution of an atom to which bonds are neither made nor broken in the rate-controlling step or in a pre-equilibrium step of a specified reaction, and is therefore not a primary isotope effect. One speaks of α, β, (etc.) secondary isotope effects, where α, β, (etc.) denote the position of isotopic substitution relative to the reaction centre. The corresponding isotope effect on the equilibrium constant of such a reaction is called a 'secondary equilibrium isotope effect'. Secondary isotope effects have been discussed in terms of the conventional electronic effects of physical organic chemistry, e.g. induction, hyperconjugation, hybridization, etc., since these properties are determined by the electron distribution, that depends on vibrationally averaged bond lengths and angles which vary slightly with isotopic substitution. While this usage is legitimate, the term 'electronic isotope effect' should be avoided, because of the misleading implication that such an effect is electronic rather than vibrational in origin.
See also: steric isotope effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1131

secondary kinetic isotope effect

See: isotope effect

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

secondary metabolites

Metabolites which are produced by routes other than the normal metabolic pathways, mostly after the phase of active growth and under conditions of deficiency. The biological significance of many secondary metabolites is not exactly known.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

secondary pollution (emissions)

The products of the primary pollutants which form through photochemical and thermal reactions in the atmosphere (O_3, peroxyacetyl nitrate, etc.).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2213

secondary radiation

Radiation emitted by any matter irradiated with electromagnetic or ionizing radiation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552

secondary structure

The conformational arrangement (α-helix, β-pleated sheet, etc.) of the backbone segments of a macromolecule such as a polypeptide chain of a protein without regard to the conformation of the side chains or the relationship to other segments.
See also: primary structure, tertiary structure, quaternary structure

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

secular equation

In molecular orbital theory, the determinant of matrix elements whose solution leads to the set of energy levels of molecular orbitals for a given system.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1962

secular equilibrium

Radioactive equilibrium where the half life of the precursor isotope is so long that the change of its activity can be ignored during the period of interest and all activities remain constant.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

sediment

The highly concentrated suspension which may be formed by the sedimentation of a dilute suspension.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

sedimentation

In the atmospheric sciences, the process of removal of an air borne particle from the atmosphere due to the effect of gravity.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2213

sedimentation coefficient, s

Velocity of sedimentation divided by the acceleration of the force field (gravitation or centrifugation).

Source:
Green Book, 2nd ed., p. 63
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 992

See also:
Purple Book, p. 62
PAC, 1994, *66*, 897 *(Quantities and units for centrifugation in the clinical laboratory (IUPAC Recommendations 1994))* on page 904

sedimentation equilibrium

The equilibrium established in a centrifugal field when there is no net flux of any component across any plane perpendicular to the centrifugal force.

Source:
Purple Book, p. 62

sedimentation field strength

The potential difference E_{sed} per unit length in a sedimentation or centrifugation cell. As the contributions of the interfacial potential differences at the electrodes are not included in E_{sed} this quantity, although theoretically important, is not accessible to measurement.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

sedimentation

in chemistry

Separation of a dispersed system under the action of a gravitational or centrifugal field according to the different densities of the components.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1825

sedimentation potential difference (sedimentation potential)

Synonym: Dorn effect

The potential difference E_{sed} or E at zero current caused by the sedimentation of particles in the field of gravity or in a centrifuge, between two identical electrodes at different levels (or at different distances from the centre of rotation). E is positive if the lower (peripheral) electrode is negative. This is also called the Dorn effect.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

sedimentation velocity method

A method by which the velocity of motion of solute component(s) or dispersed particles is measured and the result is expressed in terms of its (their) sedimentation coefficient(s).

Source:
Purple Book, p. 62

sedimentation velocity, v_{B}

Velocity of a component in a fluid relative to the fluid in the direction of gravitational or centrifugal acceleration. Also called sedimentation rate.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 992
PAC, 1994, *66*, 897 *(Quantities and units for centrifugation in the clinical laboratory (IUPAC Recommendations 1994))* on page 904

sedimentation volume

The volume V_{sed} of sediment formed in a suspension. If the sediment is formed in a centrifugal field, the strength of this field should be explicitly indicated, otherwise normal gravity is understood.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 616

segment

in analytical chemistry

1. (for bulk materials): Each of the single, large portions of material pre-existing either in space (e.g. bags, bales, drums) or accumulated during a fixed time (e.g. discharge from a conveyor belt) or formable as increments by a sampling device. Segments may be actual or conceptual.

   Source:
   PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1202
2. The set of samples which can be analysed between two successive calibrations. A segment includes samples, control materials and blank samples. This term is of particular importance in clinical chemistry.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1661

segmented copolymer

Copolymer containing phase domains of microscopic or smaller size, with the domains constituted principally of single types of structural unit.
Note:
The types of domain in a segmented copolymer usually comprise hard- and soft-segment phase domains.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2002

segregated star macromolecule

See: star macromolecule

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2296

segregation

The process that differentiates the composition at an interface or surface from the average or bulk composition.
Note:

The composition of the segregated phases need not be uniform, for example, when concentration gradients are established in the phases.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 590

segregation

in polymers

The rejection of a fraction of macromolecules, or of impurities, or both, from growing crystals. The rejected macromolecules are usually those of insufficient relative molecular mass, or differing in constitution or configuration (e.g. branching, tacticity, etc.).

Source:
Purple Book, p. 85

selected ion monitoring

in mass spectrometry

This term is used to describe the operation of the mass spectrometer in which the intensities of several specific ion beams are recorded rather than the entire mass spectrum. An alternative recommended term is multiple ion (peak) monitoring. The use of the terms multiple ion detection and mass fragmentography are not recommended, because in the case of the former, it is the monitoring of several peaks which should be emphasized rather than the detection of different ions, and in the case of the latter it is often not fragments that are being monitored but peaks from molecular ions.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1551

selection

in biotechnology

A laboratory method applying a mixture of microorganisms to particular growth conditions under which only the cells with particular characteristics can survive and may be isolated.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

selection rule

A rule that states whether a given transition is allowed or forbidden, on the basis of the symmetry or spin of the wavefunctions of the initial and final states.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273

selective corrosion

Corrosion of a single phase having more than one component, when the ratio of the corrosion rates of the components differs from the ratio of bulk mole fractions. Selective corrosion changes the composition of the material in the interfacial region.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

selective elution

in chromatography

An elution procedure in which a specific eluent is used, e.g. a complexing agent that forms stable non-sorbable complexes with one or a group of the compounds to be separated, but affects the other components only to a negligible extent.

Source:
Orange Book, p. 92

selective

in analysis

A term which expresses qualitatively the extent to which other substances interfere with the determination of a substance according to a given procedure.

Source:
PAC, 1983, *55*, 553 *(Recommendations for the usage of selective, selectivity and related terms in analytical chemistry)* on page 555

selective micro-sample

Also contains definition of: individual particle analysis

in spectrochemical analysis

A sample which results where a small portion has been separated from the lot or laboratory sample by selective means such as magnetic-, density-, or manual separation, by micro-drilling, or by centrifugation, e.g. the separation of magnetic materials from a geological material, or the separation of metal particles from a lubricating oil. If individual particles are analysed the term individual particle analysis is applied.

Source:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1467

selective poisoning

Also contains definition of: selective inhibition *in catalysis*

in catalysis

In selective poisoning or selective inhibition, a poison retards the rate of one catalysed reaction more than that of another or it may retard only one of the reactions.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 83

selective preconcentration

in trace analysis

An operation (process) as a result of which microcomponents are selectively isolated from a sample. It is used when the simultaneous presence of several components in the concentrate may distort the results of analysis. Selective preconcentration usually is achieved by isolation of the microcomponent to be determined.

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1197

selective sample

A sample that is deliberately chosen by using a sampling plan that screens out materials with certain characteristics and/or selects only material with other relevant characteristics.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1203

selective solvent

in polymer chemistry

A medium that is a solvent for at least one component of a mixture of polymers, or for at least one block of a block or graft polymer, but a non-solvent for the other component(s) or block(s).

Source:
Purple Book, p. 59

selectively labelled

An isotopically labelled compound is designated as selectively labelled when a mixture of isotopically substituted compounds is formally added to the analogous isotopically unmodified compound in such a way that the position(s) but not necessarily the number of each labelling *nuclide* is defined. A selectively labelled compound may be considered as a mixture of specifically labelled compounds.

Source:
Blue Book, p. 515
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1893

selectivity

This term is used in two different ways:

1. It sometimes refers to the discrimination shown by a given reactant A when it reacts with two alternative reactants B and C, or in two different ways (e.g. at two different sites) with a reactant B.
2. The term also sometimes refers to the ratio of products obtained from given reactants. This meaning is of importance for catalysts, which can have a wide range of selectivities. Selectivity is quantitatively expressed by ratios of rate constants for the alternative reactions, or by the decadic logarithms of such ratios.

See also: isoselective relationship, partial rate factor, regioselectivity, selectivity factor, stereoselectivity

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 186
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

selectivity coefficient, $k_{\mathrm{A/B}}$

in ion exchange chromatography

The equilibrium coefficient obtained by application of the law of mass action to ion exchange and characterizing quantitatively the ability of an ion exchanger to select one of two ions present in the same solution. The ions involved in the exchange should be specified as subscripts. Examples:
Exchange: $\mathrm{Mg}^{2+} - \mathrm{Ca}^{2+}$

$$k_{\mathrm{Mg/Ca}} = \frac{[\mathrm{Mg}]_\mathrm{S} / [\mathrm{Ca}]_\mathrm{S}}{[\mathrm{Mg}]_\mathrm{M} / [\mathrm{Ca}]_\mathrm{M}}$$

Exchange: $\mathrm{SO_4}^{2-} - \mathrm{Cl}^-$

$$k_{\mathrm{SO_4/Cl}} = \frac{[\,\mathrm{SO_4}\,]_\mathrm{S} / [\mathrm{Cl}]_\mathrm{S}^2}{[\,\mathrm{SO_4}\,]_\mathrm{M} / [\mathrm{Cl}]_\mathrm{M}^2}$$

In the above equations subscript S refers to the ion exchanger ('stationary phase') and M to the external solution ('mobile phase'). For exchanges involving counter-ions differing in their charges, the numerical value of $k_{\mathrm{A/B}}$ depends on the choice of the concentration scales in the ion exchanger and the external solution (molal scale, molar scale, mole fraction scale, etc.). Concentration units must be clearly stated for an exchange of ions of differing charges. The corrected selectivity coefficient ($k_{\mathrm{A/B}}{}^{a}$) is calculated in a way identical to the selectivity coefficient except that the concentrations in the external solutions are replaced by activities. This term should not be used as a synonym for separation factor.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 857
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2385

selectivity factor

in ion exchange chromatography

See: selectivity coefficient

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 857

selectivity factor, S_f

A quantitative representation of selectivity in aromatic substitution reactions (usually electrophilic, for monosubstituted benzene derivatives). If the partial rate factor, f, expresses the reactivity of a specified position in the aromatic compound PhX relative to that of a single position in benzene, then the selectivity factor S_f (expressing discrimination between *p*- and *m*-positions in PhX) is defined as:

$$S_f = \log_{10}\left(\frac{f_p^{\mathrm{X}}}{f_m^{\mathrm{X}}}\right)$$

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

selectivity

in analysis

1. (qualitative): The extent to which other substances interfere with the determination of a substance according to a given procedure.
2. (quantitative): A term used in conjunction with another substantive (e.g. constant, coefficient, index, factor, number) for the quantitative characterization of interferences.

Source:
PAC, 1983, *55*, 553 *(Recommendations for the usage of selective, selectivity and related terms in analytical chemistry)* on page 555

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

selectivity

of a reagent

See: selectivity factor

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1162

selectivity ratio

Synonymous with selectivity coefficient.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2386

selenenic acids

Compounds having the structure RSeOH ($R \neq H$), e.g. ArSeOH, areneselenenic acids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1364

selenides

1. Compounds having the structure RSeR ($R \neq H$). They are thus selenium analogues of ethers.
2. Metal salts of selane, H_2Se.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1364

seleninic acids

Compounds having the structure RSe(=O)OH.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

selenocyanates

Salts and esters of selenocyanic acid, HSeCN, e.g. CH_3CH_2SeCN ethyl selenocyanate.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

selenols

Compounds having the structure RSeH ($R \neq H$).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

selenones

Compounds having the structure $R_2Se(=O)_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

selenonic acids

Compounds having the structure $RSe(=O)_2OH$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

selenoxides

Compounds having the structure $R_2Se=O$ ($R \neq H$).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

self inductance, L

For a thin conducting loop, the magnetic flux through the loop, caused by an electric current in the loop, divided by that current.

Source:
Green Book, 2nd ed., p. 15
ISO 31-4: 1992

self-absorption

Occurs in emission sources of finite thickness when radiant energy quanta emitted by atoms (or molecules) are absorbed by atoms of the same kind present in the same source. The absorbed energy is usually dissipated by collisional transfer of energy, or through emission of radiant energy of the same or other frequencies. In consequence, the observed radiant intensity of a spectral line (or band component) emitted by a source may be less than the radiant intensity would be from an optically thin source having the same number of emitting atoms. Self-absorption may occur in all emitting sources to some degree, whether they are homogeneous or not.

Source:
Orange Book, p. 242
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

See also:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552
PAC, 1985, *57*, 1453 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - V: Radiation sources (Recommendations 1985))* on page 1464

self-absorption broadening

of a spectral line

Photons emitted in one region of a source are partly absorbed in their passage through the plasma. Because of the fact that the absorption profile is of the same shape as the emission profile, energy is selectively absorbed from the emission line, i.e. the absorption coefficient is a maximum at the centre of the line or central wavelength. The actual line profile is changed as a result of the lowering of the maximum intensity accompanied by a corresponding increase in apparent halfwidth.

Source:
Orange Book, p. 122

self-absorption effect

in luminescence spectroscopy

The reabsorption of luminescence by the analyte and interfering impurities within the excitation volume.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 244

self-absorption factor

Synonym: source efficiency

of a radiation source

of a radiation source

The ratio between the quantity of the radiation emitted by the source and the quantity of the radiation as produced by the radioactive nuclei present in the source. Synonymous with source efficiency.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

self-diffusion coefficient

The diffusion coefficient D_i^* of species i in the absence of a chemical potential gradient. It is related to the diffusion coefficient D_i by

$$D_i^* = D_i \frac{\partial(\ln c_i)}{\partial \ln a_i}$$

where a_i is the activity of i in the solution, and c_i is the concentration of i. If an isotopically labelled species (i^*) is used to study diffusion, the tracer diffusion coefficient, D_i^*, is practically identical to the self-diffusion coefficient provided that the isotope effect is sufficiently small.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 617

self-localized excitations
in conjugated organic polymers

Physical and chemical properties of conjugated organic polymers with π-electrons have been interpreted in terms of self-localized excitations, which are quasi-particles with structural changes over several repeating units. These excitations can be classified into *solitons*, polarons, *bipolarons* and *excitons* according to their charge and spin.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 419

self-poisoning
Synonym: autopoisoning *in catalysis*

in catalysis

A product of a reaction may cause poisoning or inhibition. The phenomenon is called self-poisoning or autopoisoning.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 83

self-quenching

Quenching of an excited atom or molecular entity by interaction with another atom or molecular entity of the same species in the ground state.
See also: Stern–Volmer kinetic relationships

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273

self-reversal

A case of self-absorption, when a line is self-absorbed to such an extent that the peak or central wavelength intensity is less than at the wings or non-central wavelengths.

Source:
Orange Book, p. 122

self-shielding

The lowering of the flux density in the inner part of an object due to absorption in its outer layers.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

selones

Compounds having the structure $R_2C{=}Se$ ($R \neq H$). They are thus selenium analogues of ketones.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

semi-empirical quantum mechanical methods

Methods which use parameters derived from experimental data to simplify computations. The simplification may occur at various levels: simplification of the Hamiltonian (*e.g.*, as in the Extended Huckel method), approximate evaluation of certain molecular integrals (see, for example, Zero differential overlap approximation), simplification of the wavefunction (for example, use of a Pi (π) electron approximation as in Pariser–Parr–Pople method), *etc*.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1962

semi-interpenetrating polymer network

Acronym: SIPN

Polymer comprising one or more polymer networks and one or more linear or branched polymers characterized by the penetration on a molecular scale of at least one of the networks by at least some of the linear or branched macromolecules.
Note:
A SIPN is distinguished from an IPN because the constituent linear or branched macromolecules can, in principle, be separated from the constituent polymer network(s) without breaking chemical bonds; it is a polymer blend.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1815

semi-rigid chain

A chain for which the contour length is greater than the persistence length but for which their ratio is still below the Gaussian limit.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 505

semicarbazones

Compounds having the structure $R_2C=NNHC(=O)NH_2$, formally derived by condensation of aldehydes or ketones with semicarbazide $[NH_2NHC(=O)NH_2]$.

Source:
PAC, 1996, *68*, 1361 *(Functional dyes from nature: Potentials for technical applications)* on page 1365

semicoke

A carbonaceous material intermediate between a fusible mesophase pitch and a non-deformable green coke produced by incomplete carbonization at temperatures between the onset of fusion (of coal, *ca.* 620 K), and complete devolatilization. Semicoke still contains volatile matter, therefore.
Note:
Semicoke may be conceived as covering a continuous range from coal that has not yet been fused to coke breeze. Semicoke can also be used as a filler in carbon mixtures.
See also: coal tar pitch

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 504

semiconductor

Material whose conductivity, due to charges of both signs, is normally in the range between that of metals and insulators and in which the electric charge carrier density can be changed by external means.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552

semiconductor detector

A radiation detector using a semiconductor, in which free electric charges are produced along the path of an ionizing particle, in combination with a high voltage and electrodes to collect the induced electric charges.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

See also:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1754

semiconductor laser [obsolete]

Usage not recommended.
See: diode laser

Source:
PAC, 1995, *67*, 1913 *(Nomenclature, symbols, units, and their usage in spectrochemical analysis-XV. Laser-based molecular spectroscopy for chemical analysis - laser fundamentals (IUPAC Recommendations 1995))* on page 1920

semiconductor-metal transition

Any transition from a semiconductor to a metallic state under the influence of a temperature or pressure change or both. Examples:

1. Ti_2O_3: band-edge crossing in a semiconductor to semimetal transition.
2. SmS: localized level crossing a band edge. In SmS hydrostatic pressure above the critical pressure $P_c \approx 0.65$ GPa broadens the Sm-5d band to make the band edge cross the Sm-$4f^6$ level.
3. A localized-itinerant transition.
4. A switching transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 590

semioxamazones

Compounds having the structure $R_2C{=}NNHC({=}O)C({=}O)NH_2$, formally derived from the condensation of aldehydes or ketones with semioxamazide (the hydrazide of oxamic acid), $H_2NNHC({=}O)C({=}O)NH_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

semiquinones

Radical anions having the structure $O^{-}{-}Z{-}O^{\cdot}$ where Z is an *ortho*- or *para*-arylene group or analogous heteroarylene group; they are formally generated by the addition of an electron to a quinone.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

semisystematic name (semitrivial name)

A name in which at least one part is used in a systematic sense.

Source:
Blue Book (Guide), p. 14

seniority (senior)

in organic nomenclature

Terms used in reference to priority in a prescribed hierarchical order, a senior feature being preferred.

Source:
Blue Book (Guide), p. 17

sensitive area

of a radiation detector

That area of the detector where an incident radiant power results in a measurable output.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1751

sensitive volume

of a radiation detector

That volume of the detector where an incident radiant power produces a measurable output.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1751

sensitivity

in mass spectrometry

Two different measures of sensitivity are recommended. The first, which is suitable for relatively involatile materials as well as gases, depends upon the observed change in ion current for a particular amount or change of flow rate of sample though the ion source. A second method of stating sensitivity, that is most suitable for gases, depends upon the change of ion current related to the change of partial pressure of the sample in the ion source. It is important that the relevant experimental conditions corresponding to sensitivity measurement should always be stated. These include in a typical case details of the instrument type, bombarding electron current, slit dimensions, angular collimation, gain of the multiplier detector, scan speed and whether the measured signal corresponds to a single mass peak or to the ion beam integrated over all masses. Some indication of the time involved in the determination should be given, e.g. counting time or band width. The sensitivity should be differentiated from the detection limit.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1553
Orange Book, p. 206

sensitivity, A

in metrology and analytical chemistry

The slope of the calibration curve. If the curve is in fact a 'curve', rather than a straight line, then of course sensitivity will be a function of analyte concentration or amount. If sensitivity is to be a unique performance characteristic, it must depend only on the chemical measurement process, not upon scale factors.

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1703
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

See also:
Orange Book, p. 5
Orange Book, p. 36

sensitization

See: photosensitization

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273

sensitization

in colloid chemistry

Addition of small amounts of a hydrophilic colloid to a hydrophobic sol to possibly make the latter more sensitive to flocculation by electrolyte.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 610

sensitized luminescence

The deactivation of the primarily excited emitter which can lead to the activation of the quencher followed by radiative deactivation.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 235

sensitizer

See: photosensitizer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273

separability assumption

This expression refers to the assumption, essential to conventional transition-state theory, that the energy of the system may be expressed as the sum of components associated with different degrees of freedom. In transition-state theory it is assumed that the energy of the motion of the system through the dividing surface of the potential-energy surface is separable into various components. In many practical calculations it is assumed that the energy of the system is separable into electronic, vibrational, rotational and translational energy.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 186

separated flame

Also contains definition of: shielded flame *in flame spectroscopy*

in flame spectroscopy

In a premix burner, sometimes provision is made to screen the observed portion of the flame gases from direct contact with the surrounding air. This may be done either mechanically by placing a tube on top of the burner around the flame, which produces a zonal separation (separated flame), or aerodynamically by surrounding the flame with a sheath of inert gas that emerges from openings at the rim of the burner top (shielded flame).

Source:
Orange Book, p. 166

separation coefficient [obsolete]

Synonymous with separation factor. Use of this term is not recommended.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2386

separation factor, α

in column chromatography

The relative retention value calculated for two adjacent peaks ($V'_{\mathrm{R}\,2} > V'_{\mathrm{R}\,1}$):

$$\alpha = \frac{V'_{\mathrm{R}\,2}}{V'_{\mathrm{R}\,1}} = \frac{V_{\mathrm{N}\,2}}{V_{\mathrm{N}\,1}} = \frac{t'_{\mathrm{R}\,2}}{t'_{\mathrm{R}\,1}} = \frac{k_2}{k_1}$$

By definition, the value of the separation factor is always greater than unity. The separation factor is also identical to the ratio of the corresponding distribution constants. The separation factor is sometimes also called the 'selectivity'. The use of this expression is discouraged.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 844

separation factor, $\alpha_{\mathrm{A,B}}$

in liquid-liquid distribution

The ratio of the respective distribution ratios of two extractable solutes measured under the same conditions.

$$\alpha_{\mathrm{A,B}} = \frac{D_{\mathrm{A}}}{D_{\mathrm{B}}}$$

Notes:

1. By convention the solutes designated as A and B in the above are chosen so as to make $\alpha > 1$.
2. The term separation coefficient is not recommended.
3. The terms selectivity coefficient and selectivity ratio are not synonymous and should not be used.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2386
Orange Book, p. 107

See also:
Orange Book, p. 85

separation number, SN

in chromatography

This expresses the number of peaks which can be resolved in a given part of the chromatogram between the peaks of two consecutive *n*-alkanes with z and $(z + 1)$ carbon atoms in their molecules:

$$\mathrm{SN} = \frac{t_{\mathrm{R}\,(z+1)} - t_{\mathrm{R}\,z}}{w_{\mathrm{h}\,z} + w_{\mathrm{h}\,(z+1)}} - 1$$

In the German literature the symbol TZ (trennzahl) is commonly used to express the separation number. As the separation number depends on the *n*-alkanes used for the calculation, they always must be specified with any given SN value.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 847

separation temperature

in chromatography

The temperature of the chromatographic bed under isothermal operation. In column chromatography it is called the column temperature.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 838

sequence

The order of neighbouring amino acids in a protein or of the purine or pyrimidine bases in RNA or DNA.
See also: primary structure

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1296

sequence rules

See: priority

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

sequencing (proteins, nucleic acids)

Analytical procedures for the determination of the order of amino acids in a polypeptide chain or of nucleotides in a DNA or RNA molecule.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

sequential analyser

A discontinuous analyser in which at least one sub-assembly operates sequentially.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

sequential indication

of an analyser

An indication obtained following sequential sampling or received from a sequential cell or from data processing comprising a succession of predetermined repetitive operations (or a combination of the three).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2174

sequential interpenetrating polymer network

Interpenetrating polymer network prepared by a process in which the second component network is formed following the formation of the first component network.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1814

sequential measuring cell

A measuring cell which operates according to a succession of operations on the sample or on the sensitive elements (or on both), these operations being carried out according to one or more repetitive programs.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2178

sequential sample

Units, increments or samples taken one at a time or in successive predetermined groups, until the cumulative result of their measurements (typically applied to attributes), as assessed against predetermined limits, permits a decision to accept or reject the population or to continue sampling. The number of observations required is not determined in advance, but the decision to terminate the operation depends, at each stage, on the results of the previous observations. The plan may have a practical, automatic termination after a certain number of units have been examined.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1203

sequential semi-interpenetrating polymer network

Semi-interpenetrating polymer network prepared by a process in which the linear or branched components are formed following the completion of the reactions that lead to the formation of the network(s) or *vice versa*.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1815

sequential spectrometer

A spectrometer which enables the intensity of several spectral bands of radiation to be measured one after the other in time, i.e. sequentially.

Source:
PAC, 1995, *67*, 1725 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-IX. Instrumentation for the spectral dispersion and isolation of optical radiation (IUPAC Recommendations 1995))* on page 1729

series

of analytical results

A number of measured values (x_1, x_2, ... x_i, ... x_n) equivalent to each other with respect to statistical considerations, e.g. the results of repeated analyses using only one analytical method on a substance that is presumed to be homogeneous.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 597
Orange Book, p. 4

serum

1. Watery proteinaceous portion of the blood that remains after clotting. Synonym: blood serum
2. Clear watery fluid especially that moistening the surface of serous membranes or that exuded through inflammation of any of these membranes.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1070

sesquiterpenoids

Terpenoids having a C_{15} skeleton.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

sesterterpenoids

Terpenoids having a C_{25} skeleton. Sometimes erroneously referred to as sesterpenoids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

settling chamber

in atmospheric chemistry

Chamber designed to reduce the velocity of gases in order to permit the settling out of fly ash. It may be either part of, adjacent to, or external to an incinerator.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2213

settling error

in spectrochemical analysis

An error caused by allowing insufficient time for the reading to settle or if an absorption peak is scanned too rapidly.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1456

settling velocity

The terminal rate of fall of a particle through a fluid as induced by gravity or other external force.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2213

shape selectivity

in catalysis

Possibly observed in catalysts with very small pores. The selectivity is largely determined by the bulk or size of one or more reactants.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 81

shape-memory polymer

Polymer that, after heating and being subjected to a plastic deformation, resumes its original shape when heated above its glass-transition or melting temperature.
Note:
Crystalline *trans*-polyisoprene is an example of a shape-memory polymer.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 903

shear dependent viscosity

For systems showing non-Newtonian behaviour when measured in steady simple shear, a coefficient η equal to $\frac{\sigma}{D}$ at a given value of the shear rate D, where σ is the stress; η_0 is the limiting viscosity at zero shear rate, and η_∞ the limiting viscosity at infinite shear rate; $[\,\eta_0\,]$ is the limit of intrinsic viscosity at zero shear.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

shear modulus, G

Shear stress divided by shear strain.

Source:
Green Book, 2nd ed., p. 12

shear rate

The velocity gradient in a flowing fluid.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

shear strain, γ

Displacement of one surface with respect to another divided by the distance between them.

Source:
Green Book, 2nd ed., p. 12

shear stress, τ

Force acting tangentially to a surface divided by the area of the surface.

Source:
Green Book, 2nd ed., p. 12

shear thinning

Also contains definition of: shear thickening

If viscosity is a univalued function of the rate of shear, a decrease of the viscosity with increasing rate of shear is called shear thinning, and an increase of the viscosity shear thickening.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

shear transition

A diffusionless transition that involves a change of the shape of the unit cell by a process that can be described as shear.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 590

shear viscosity

For a Newtonian fluid, the shear viscosity is often termed simply viscosity since in most situations it is the only one considered. It relates the shear components of stress and those of rate of strain at a point in the fluid by:

$$\sigma_{xy} = \sigma_{yx} = \eta \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) = 2\, \eta\, \dot{\gamma}_{yx}$$

where $\dot{\gamma}_{yx}$, the shear component of rate of strain is defined as follows:

$$\dot{\gamma}_{yx} = \frac{1}{2} \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right)$$

Corresponding relations hold for σ_{xz} and σ_{yz}; σ_{xy} is the component of stress acting in the y-direction on a plate normal to the x-axis; v_x, v_y, v_z are the components of velocity.
See also: shear dependent viscosity

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1216

shielding

Also contains definition of: deshielding

In the context of NMR spectroscopy shielding is the effect of the electron shells of the observed and the neighbouring nuclei on the external magnetic field. The external field induces circulations in the electron cloud. The resulting magnetic moment is oriented in the opposite direction to the external field, so that the local field at the central nucleus is weakened, although it may be strengthened at other nuclei (deshielding). The phenomenon is the origin of the structural dependence of the resonance frequencies of the nuclei.
See also: chemical shift

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1163

shielding constant, σ

In NMR the difference between the external magnetic flux density and the local magnetic flux density at a resonating nucleus affected by the neighbouring electrons divided by the external flux density, $\sigma = \frac{B_0 - B}{B_0}$.

Source:
Green Book, 2nd ed., p. 25

shish-kebab structure

A polycrystalline morphology of double habit consisting of fibrous crystals overgrown epitaxially by lamellar crystals, the stems of which are parallel to the fibre axis.

Source:
Purple Book, p. 83

short chain

A chain of low relative molecular mass.
See: oligomer molecule (1)

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2294

short-range intramolecular interactions

in polymers

A steric or other interaction involving atoms or groups or both situated nearby in sequence along the chain. The interacting atoms or groups are typically separated by fewer than ten consecutive bonds in a chain. If no confusion can occur, the word 'intramolecular' may be omitted.

Source:
Purple Book, p. 48

shrinkage

Decrease in volume of a network, gel or solid associated with the exudation of a fluid.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1825

shut-down state

in analysis

The condition of an instrument when it is switched off to conserve energy or reagents or to protect working parts. This term is of particular importance in clinical chemistry.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1664

shut-down time

in analysis

The time interval between production of the last result of an instrument and shut-down state.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1664

shuttle vector

A DNA molecule (e.g. plasmid) that is able to replicate in two different host organisms and can therefore be used to 'shuttle' or convey genes from one to the other.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 165

SI

Synonym: International system of units

Système International d'Unités, the international system of units established in 1960 and based on seven base units for the quantities: length, time, mass, electric current, thermodynamic temperature, amount of substance and luminous intensity.

Source:
Green Book, 2nd ed., p. 69

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 995

sialon

A generic name for compounds or solid solutions in the system M–Si–Al–O–N where M is a metal. (The use of capitals as in SiAlON is discouraged since they suggest a chemical composition.)

Source:
PAC, 1999, *71*, 1765 *(Terminology for compounds in the Si-Al-O-N system)* on page 1767

side group or side-chain polymer liquid crystal

A polymer, the molecules of which have mesogenic units only in side-group's side-chains.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 503

siemens

SI derived unit of electric conductance, $\mathrm{S} = \Omega^{-1} = \mathrm{m}^{-2}\,\mathrm{kg}^{-1}\,\mathrm{s}^{3}\,\mathrm{A}^{2}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 992

sievert

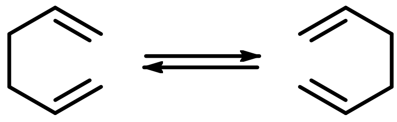
SI derived unit of dose equivalent (the mean specific energy imparted to an element of matter corrected by a quality factor and a modifying factor to take into account the properties of irradiated matter) equal to one joule per kilogram and admitted for reasons of safeguarding human health.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 992

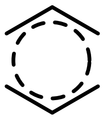
sigmatropic rearrangement

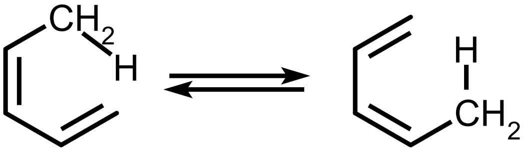
A molecular rearrangement that involves both the creation of a new σ-bond between atoms previously not directly linked and the breaking of an existing σ-bond. There is normally a concurrent relocation of π-bonds in the molecule concerned, but the total number of π- and σ- bonds does not change. The term was originally restricted to intramolecular pericyclic reactions, and many authors use it with this connotation. It is, however, also applied in a more general, purely structural, sense. If such reactions are intramolecular, their transition state may be visualized as an association of two fragments connected at their termini by two partial σ-bonds, one being broken and the other being formed as, for example, the two allyl fragments in (a'). Considering only atoms within the (real or hypothetical) cyclic array undergoing reorganization, if the numbers of these in the two fragments are designated i and j, then the rearrangement is said to be a sigmatropic change of order $[i, j]$ (conventionally $[i] \leq [j]$). Thus the rearrangement (a) is of order [3,3], whilst reaction (b) is a [1,5]sigmatropic shift of hydrogen. (N.B. By convention square brackets [...] here refer to numbers of atoms, in contrast with current usage in the context of cycloaddition.)

(a)

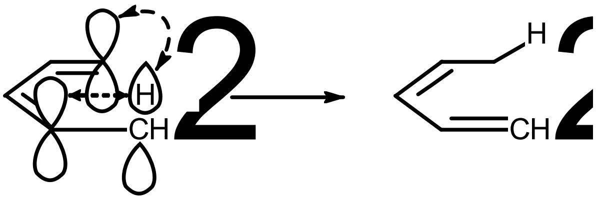


(a')



(b) 

The descriptors a and s (antarafacial and suprafacial) may also be annexed to the numbers *i* and *j*; (b) is then described as a [1s,5s] sigmatropic rearrangement, since it is suprafacial with respect both to the hydrogen atom and to the pentadienyl system:



The prefix 'homo' (meaning one extra atom, interrupting conjugation — *cf.* 'homoaromaticity') has frequently been applied to sigmatropic rearrangements, but is misleading.
See also: cycloaddition, tautomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1163

signal

in analysis

A representation of a quantity within an analytical instrument.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1662

silanes

Saturated silicon hydrides, analogues of the alkanes; i.e. compounds of the general formula Si_nH_{2n+2}. Silanes may be subdivided into silane, oligosilanes and polysilanes. Note hydrocarbyl derivatives and other derivatives are often referred to loosely as silanes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

silanols

1. In a strict sense, hydroxy derivatives of silanes $Si_nH_{2n+1}OH$.
2. A name commonly applied to Si-hydrocarbyl derivatives, R_3SiOH, of silanol, H_3SiOH.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1365

silasesquiazanes

Compounds in which every silicon atom is linked to three nitrogen atoms and every nitrogen atom is linked to two silicon atoms, thus consisting of SiH and NH units, and having the general formula $(SiH)_{2n}(NH)_{3n}$. By extension hydrocarbyl derivatives are commonly included.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

silasesquioxanes

Compounds in which every silicon atom is linked to three oxygen atoms and every oxygen atom is linked to two silicon atoms, and having the general formula $(SiH)_{2n}O_{3n}$. By extension hydrocarbyl derivatives are commonly included.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

silasesquithianes

Compounds in which every silicon atom is linked to three sulfur atoms and every sulfur atom is linked to two silicon atoms, and having the general formula $(SiH)_{2n}S_{3n}$. By extension hydrocarbyl derivatives are commonly included.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

silathianes

Compounds having the structure $H_3Si[SSiH_2]_nSSiH_3$ and branched-chain analogues. They are analogous in structure to siloxanes with –S– replacing –O–. By extension hydrocarbyl derivatives are commonly included.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

silazanes

Saturated silicon-nitrogen hydrides, having straight or branched chains. They are analogous in structure to siloxanes with –NH– replacing –O– , e.g. $H_3SiNHSiH_2NHSiH_3$ trisilazane. By extension hydrocarbyl derivatives are commonly included.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

silicones

Polymeric or oligomeric siloxanes, usually considered unbranched, of general formula $[–OSiR_2–]_n$ $(R \neq H)$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

siloxanes

Saturated silicon-oxygen hydrides with unbranched or branched chains of alternating silicon and oxygen atoms (each silicon atom is separated from its nearest silicon neighbours by single oxygen atoms). The general structure of unbranched siloxanes is $H_3Si[OSiH_2]_nOSiH_3$. $H_3Si[OSiH_2]_nOSiH[OSiH_2OSiH_3]_2$ is an example of a branched siloxane. By extension hydrocarbyl derivatives are commonly included.
See also: silicones

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

silver film

When viewed in reflected white light against a black background, transparent films show the classical interference colours of thin plates which permit an estimate of their thickness to be made. When of the order of $100\ \mathrm{nm}$ $(1000\ \mathrm{Å})$ in thickness they appear white (silver film) and when thinner they appear gradually less intensely white, then grey and finally black.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 614

silyl groups

1. In a strict sense, the silyl group is $H_3Si–$.
2. A name commonly applied to hydrocarbyl derivatives of the silyl group $R_3Si–$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

silyl radicals

1. In a strict sense, the silyl radical is $H_3Si^{\cdot}$.
2. A name commonly applied to the silicon-centered radicals $R_3Si^{\cdot}$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

silylene

1. Generic name for H_2Si: and substitution derivatives thereof, containing an electrically neutral bivalent silicon atom with two non-bonding electrons. (The definition is analogous to that given for carbene.)
2. The silanediyl group (H_2Si), analogous to the methylene group (H_2C).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1164

simple shear

An idealized treatment of a fluid between two large parallel plates (to permit ignoring edge effects) of area A, separated by a distance h. If one plate moves relative to the other with a constant velocity V, requiring a force F acting in the direction of movement, and the density, pressure, and viscosity throughout the fluid are constant, the Newtonian equation can be coupled with the equations of motion and of continuity to show that the velocity gradient in the fluid is constant ($= \frac{V}{h}$), and that $\frac{F}{A} = \frac{\eta\, V}{h}$. This idealized case (simple shear) is sometimes used to define shear viscosity.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1216

simulation technique

in analysis

A technique for reducing or eliminating analytical errors resulting from interferences, using a reference solution sufficiently similar in quantitative composition to the sample solutions to be analysed that the interferences in the reference and sample solution are equivalent.

Source:
Orange Book, p. 172

simultaneous interpenetrating polymer network

Interpenetrating polymer network prepared by a process in which the component networks are formed concurrently.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1814

simultaneous pair transitions

Simultaneous electronic transitions in two coupled absorbers or emitters. Because of the coupling, transitions which are spin-forbidden in one of the centres might become spin-allowed (spin flip).

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273

simultaneous reactions

Composite reactions, in which processes like

$$\mathrm{A} \overset{1}{\rightarrow} \mathrm{Y}$$

and

$$\mathrm{B} \overset{2}{\rightarrow} \mathrm{Z}$$

occur in parallel, can be called simultaneous or parallel reactions. Sometimes there is competition involved, like in the scheme:

$$\mathrm{A} + \mathrm{B} \overset{1}{\rightarrow} \mathrm{Y}$$

and

$$\mathrm{A} + \mathrm{C} \overset{2}{\rightarrow} \mathrm{Z}$$

where B and C compete with one another for A.

Source:
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2297

simultaneous semi-interpenetrating polymer network

Semi-interpenetrating polymer network prepared by a process in which the networks and the linear or branched components are formed concurrently.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1816

simultaneous spectrometer

A spectrometer which has more than one detector and enables the intensities of several spectral bands to be measured at the same time.

Source:
PAC, 1995, *67*, 1725 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-IX. Instrumentation for the spectral dispersion and isolation of optical radiation (IUPAC Recommendations 1995))* on page 1729

single cell protein (SCP)

Microbial biomass or proteins extracted therefrom obtained from processes in which bacteria, yeasts, other fungi or algae are cultivated in large quantities as human or animal protein supplement in animal feed or in human nutrition.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 166

single escape peak

In a γ-ray spectrum, the peak due to pair production in the detector and escape, from the sensitive part of the detector, of one of the photons of $511\ \mathrm{keV}$ resulting from annihilation.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

single scattering

Radiation scattering in which there is only one scattering encounter.
See also: light scattering

Source:
PAC, 1983, *55*, 931 *(Definitions, terminology and symbols in colloid and surface chemistry. Part 1.14: Light scattering (Provisional))* on page 932

single-beam (luminescence) spectrometer

A luminescence spectrometer in which a single beam of radiation is used for excitation and a single beam of luminescence radiation is taken from the sample.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 238

single-electron transfer mechanism (SET)

A reaction mechanism characterized by the transfer of a single electron between the species occurring on the reaction coordinate of one of the elementary steps.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1164

single-focusing mass spectrometer

An instrument in which an ion beam with a given value of mass/charge is brought to a focus although the initial directions of the ions diverge.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546
Orange Book, p. 201

single-photon timing

Technique that permits recovery of the parameters characterizing a fluorescence decay after pulse excitation (in particular excited-states lifetimes). It is based on the creation of a time histogram of many stochastic events involving the time delay between the electronic excitation of a molecule or material and its emission of a photon from an excited state. A key to the technique is that no more than one photon strike the detector per pulsed excitation. Excitation is commonly achieved with a flash from a repetitive nanosecond lamp or diode laser or a CW operated laser (mode-locked laser). The essential components of the hardware are a device to measure the excitation-emission delay time and another to determine the relative frequency of photons reaching the detector at each delay time. Delay times are usually measured with a time-to-amplitude-converter (TAC), using voltage to measure the delay between a start and a stop signal. The frequency of events with each delay is stored in a multi-channel analyser. This term is preferred to time-correlated single-photon counting.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 420

single-step reaction

A reaction that proceeds through a single transition state.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1164

single-strand chain

in a polymer

A chain that comprises constitutional units connected in such a way that adjacent constitutional units are joined to each other through two atoms, one on each constitutional unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2294

single-strand macromolecule

A macromolecule that comprises constitutional units connected in such a way that adjacent constitutional units are joined to each other through two atoms, one on each constitutional unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2294

single-strand polymer

A polymer the macromolecules of which are single-strand macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2303

singlet molecular oxygen (singlet molecular dioxygen)

Oxygen molecule (dioxygen), O_2, in an excited singlet state. The ground state of O_2 is a triplet ($^3\Sigma_g^-$). The two metastable singlet states derived from the ground-state configuration are $^1\Delta_g$ and $^1\Sigma_g^+$ (the latter with the higher energy).
Notes:

1. Use of the term singlet oxygen alone, without mention of the chemical species is discouraged since it can also refer to an oxygen atom in a ^1S or ^1D excited state. The oxygen atom ground state is a triplet ^3P state and the ^1S and ^1D states are also derived from the ground-state configuration.
2. Triplet state quenching by triplet dioxygen (i.e., a process of photosensitization) is the most common procedure for the production of singlet molecular dioxygen in solution. For many

chemical species, the efficiency with which the triplet state is quenched by triplet dioxygen and, independently, the efficiency with singlet molecular dioxygen is produced, is controlled by the spin-statistical factor.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 420

singlet state

A state having a total electron spin quantum number equal to 0.
See: multiplicity

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273

singlet-singlet absorption

Absorption which results in the transition from the singlet ground state of the molecule into singlet excited states ($S_0 \rightarrow S_n$) and leads to the UV/visible absorption spectrum.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 234

singlet-singlet annihilation

See: annihilation, spin conservation rule

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273

singlet-singlet energy transfer

Transfer of excitation from an electronically excited donor in a singlet state to produce an electronically excited acceptor in a singlet state.
See: electron exchange excitation transfer, Förster excitation transfer, radiative energy transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273

singlet-triplet absorption

Absorption which takes place with the transition from the singlet ground state of the molecule to triplet states ($S_0 \rightarrow T_n$) and results in the singlet-triplet absorption spectrum.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 234

singlet-triplet energy transfer

Transfer of excitation from an electronically excited donor in a singlet state to produce an electronically excited acceptor in a triplet state.
See: energy transfer, spin conservation rule

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2273

singlet–triplet crossing

Point of intersection between the potential energy surfaces of states of different multiplicity.
Note:
The intersection belongs to a $(3\,N-7)$-dimensional subspace of the $(3\,N-6)$-dimensional nuclear coordinate space and therefore appears as a line on a two-dimensional energy surface (N is the number of nuclei). In this case the branching plane is one-dimensional and is defined by the gradient difference vector $\boldsymbol{x}_1$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 421

singly labelled

A specifically labelled compound in which the isotopically substituted molecule has only one isotopically modified atom e.g. $CH_3–CH[^2H]–OH$.

Source:
Blue Book, p. 515
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1892

sink

in atmospheric chemistry

The receptor for material which is removed from the atmosphere. Because of long range transport of many pollutants such as SO_2, sulfuric acid and its salts, the sink region can be many hundreds of kilometres from the source region of the pollutants.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2213

sintering

Temperature-induced coalescence and densification of porous solid particles below the melting points of their major components.
Notes:

1. The term was originally coined for the process by which fly ash produced in combustion of fuels such as coal is baked at a very high temperature. The sintered material is used in the manufacture of cinder blocks and other ceramic products.
2. Modified from previous definition. The definition proposed here is recommended as being more explicit.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1825

size-exclusion chromatography (SEC)

A separation technique in which separation mainly according to the hydrodynamic volume of the molecules or particles takes place in a porous non-adsorbing material with pores of approximately the same size as the effective dimensions in solution of the molecules to be separated.

Source:
Purple Book, p. 69

skeletal atom

An atom of a skeletal structure.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2296

skeletal bond

A bond connecting two skeletal atoms.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2296

skeletal structure

The sequence of atoms in the constitutional unit(s) of a macromolecule, an oligomer molecule, a block or a chain which defines the essential topological representation.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2296

skew

See: torsion angle, chair, boat, twist

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

Slater determinant

The determinantal representation of many-electron wavefunction Ψ which conforms to the requirement of the antisymmetry principle.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1962

Slater-type orbital

An approximate atomic orbital attempts to allow for electron-electron repulsion by scaling the nuclear charge for each orbital.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1164

slip

Ceramic precursor dispersed in a liquid.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1805

slip casting

Procedure in ceramic processing whereby slip is contained in a porous plaster mould prior to pyrolysis.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1825

slow neutrons

Neutrons of kinetic energy less than some specified value. This value may vary over a wide range and depends on the application. In reactor physics, the value is frequently chosen to be $1\ \mathrm{eV}$; in dosimetry, the effective cadmium cut-off is used.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1547

SM-interference

Interference by a substance that produces a signal by a similar mechanism to the analyte, which in the given procedure (including the apparatus used) can not be distinguished from the signal given by the analyte. For example, in a colour reaction with an organic ligand by also reacting with the ligand and producing a coloured compound absorbing at the same wavelength as the compound produced by the analyte or in an atomic spectrochemical analysis by absorbing or emitting at the same wavelength as the analyte.

Source:
PAC, 1983, *55*, 553 *(Recommendations for the usage of selective, selectivity and related terms in analytical chemistry)* on page 554

small particle

in radiation scattering

A particle much smaller than the wavelength of the radiation in the medium. In practice, all dimensions of a particle considered small must be less than about one-twentieth of the wavelength employed.

Source:
Purple Book, p. 65

smectic state

See: liquid-crystal transitions, mesomorphic phase

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 590
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

SMILES

SMILES (Simplified Molecular Input Line Entry System) is a string notation used to describe the nature and topology of molecular structures.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1150

smog chamber

in atmospheric chemistry

A large confined volume in which sunlight or simulated sunlight is allowed to irradiate air mixtures of atmospheric trace gases (hydrocarbons, nitrogen oxides, sulfur dioxide, etc.) which undergo oxidation. In theory these chambers allow the controlled study of complex reactions which occur in the atmosphere. However, ill-defined wall reactions which generate some molecular and radical species (e.g. HONO, CH_2O, HO-radicals, etc.) and remove certain products (H_2O_2, HNO_3, etc.), the use of reactant concentrations well above those in the atmosphere, ill-defined light intensities and wavelength distribution within the chamber, and other factors peculiar to chamber experiments require that caution be exercised in the extrapolation of results obtained from them to atmospheric systems.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2214

smog

in atmospheric chemistry

The term originated in Great Britain as a popular derivation of 'smoke-fog' and appears to have been in common use before World War 1. It originally referred to the heavy pollution derived largely from coal burning (largely smoke filled air, rich in sulfur dioxide), and it probably was largely a reducing atmosphere. More common today in cities is an oxidizing atmosphere which contains ozone and other oxidants.
See: photochemical smog

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2214

smog index

in atmospheric chemistry

A mathematical correlation between smog and meteorological and/or pollutant concentrations associated with it. These are qualitative indices which are sometimes used in some urban communities to predict the degree of the air pollution which is expected for the coming day.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2214

smoke

An aerosol originating from combustion, thermal decomposition or thermal evaporation. Its particles may be solid (magnesium oxide smoke) or liquid (tobacco smoke).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 606

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2214

soap

Also contains definition of: neat soap

A salt of a fatty acid, saturated or unsaturated, containing at least eight carbon atoms or a mixture of such salts. A neat soap is a lamellar structure containing much (e.g. 75%) soap and little (e.g. 25%) water.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

soap curd

A gel-like mixture of fibrous soap-crystals ('curd-fibres') and their saturated solution (not a mesomorphic phase).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

soap film

A term established by usage for A/W/A films stabilized by surfactants although it is not a film of soap, nor is the stabilizing surfactant necessarily a soap. (A/W/A means water film in air).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

soft-segment phase domain

Phase domain of microscopic or smaller size, usually in a block, graft, or segmented copolymer, comprising essentially those segments of the polymer that have glass transition temperatures lower than the temperature of use.
Note:

Soft-segment phase domains are often larger than hard-segment phase domains and are often continuous.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 2002

soiling

in atmospheric chemistry

Visible damage to materials by deposition of air pollutants.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2214

sol

A fluid colloidal system of two or more components, e.g. a protein sol, a gold sol, an emulsion, a surfactant solution above the critical micelle concentration.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 606

sol fraction

Mass fraction of the dissolved or dispersed material, resulting from a network-forming polymerization or crosslinking process, that is constituted of molecules of finite (statistically definable) relative molecular masses.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1806

sol-gel coating

Coating formed through a sol-gel process.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1818

sol-gel critical concentration

Also contains definition of: critical concentration

Concentration of an added electrolyte above which a particulate sol undergoes coagulation instead of gelation.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1825

sol-gel material

Material formed through a sol-gel process.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1818

sol-gel metal oxide

Metal oxide formed through a sol-gel process.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1818

sol-gel process

Process through which a network is formed from solution by a progressive change of liquid precursor(s) into a sol, to a gel, and in most cases finally to a dry network.
Note:
An inorganic polymer, e.g., silica gel, or an organic–inorganic hybrid can be prepared by sol-gel processing.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1825

sol-gel silica

Silica formed through a sol-gel process.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1818

sol-gel transition

Transition of a sol to a gel at the gel point.
Note:
Corrected from previous definition, within which the definition improperly attempts a redefinition of the terms sol and gel. The definition proposed here is recommended for its precision through cross-reference to the properly defined terms.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1826

solar conversion efficiency

The ratio of the Gibbs energy gain per unit time per m^2 of surface exposed to the sun and the solar irradiance, E, integrated between $\lambda = 0$ and $\lambda = \infty$.
See also: photoelectrolytic cell

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2274

solar flare

A bright eruption of energy from the sun's chromosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

solar radiation

in atmospheric chemistry

The electromagnetic radiation emitted by the sun. The total range of wavelengths of light emitted by the sun (99.9% in the range from 150 to $4000\ \mathrm{nm}$) is filtered on entering the earth's atmosphere, largely through the absorption by oxygen, ozone, water vapour and carbon dioxide. Near sea level only light of wavelengths longer than about $290\ \mathrm{nm}$ is present. The light from $290 – 400\ \mathrm{nm}$ is effective in inducing important photochemical processes since absorption by the important trace gases, ozone, nitrogen dioxide, aldehydes, ketones, etc., is significant in this region.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2214

solid angle, Ω, ω

Of a cone, the ratio of the area cut out on a spherical surface (with its centre at the apex of that cone) to the square of the radius of the sphere. It is a quantity of dimension one (dimensionless quantity) with unit steradian ($\mathrm{sr} = 1$).

Source:
Green Book, 2nd ed., p. 11
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 992

solid phase antibody radioimmunoassay

A kind of radioimmunoassay employing an antibody bound to a solid phase.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2524

solid polymer electrolyte

Electrically conducting solution of a salt in a polymer.
Notes:

1. An example of a solid polymer electrolyte is a solution of a lithium salt in a poly(oxyethylene) matrix; the ionic conductivity of such material is due to the mobility of lithium cations and their counterions in an electric field.
2. Although the adjective 'solid' is used, the material may be a liquid.
3. The term solid polymer electrolyte should not be confused with the term polymeric electrolyte.
4. ***See also:*** conducting polymer composite.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2073

solid state lasers

CW or pulsed lasers in which the active medium is a solid matrix (crystal or glass) doped with an ion (e.g. Nd^{3+} , Cr^{3+} , Er^{3+}). The emitted wavelength depends on the active ion, the selected optical transition, and the matrix. Some of these lasers are tunable within a very broad range (e.g. from 700 to $1000\ \mathrm{nm}$ for Ti^{3+} doped sapphire). Pulsed lasers may be free-running, Q-switched, or mode-locked. Some CW lasers may be mode-locked.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2274

solid support

in column chromatography

Normally an inert porous solid, which sorbs the liquid phase. The particle-size range of the support affects column efficiency and the pressure differential necessary to achieve a given flow rate. Modifications have been introduced for the achievement of special separations, in which the solid support is not inert but is an active solid. In capillary columns the inner wall of the column serves as the solid support and obviates the use of additional porous solids for this purpose.

Source:
Orange Book, p. 98
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 830

solid volume

in column chromatography

The volume occupied by the solid or the active solid in the column.

Source:
Orange Book, p. 98

solidification

The transition of a liquid or gas into a solid.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 590

solidus

A line on a binary phase diagram (or a surface on a ternary phase diagram) that indicates the temperature at which a system becomes completely solid on cooling or at which melting begins on heating under equilibrium conditions.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 590

soliton

Localized excitations propagating in a system with constant velocity and colliding with each other without change in their shapes.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 422

solubility

The analytical composition of a saturated solution, expressed in terms of the proportion of a designated solute in a designated solvent, is the solubility of that solute. The solubility may be expressed as a concentration, molality, mole fraction, mole ratio, etc.

Source:
Orange Book, p. 84

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2214

solubility parameter, δ

Parameter used in predicting the solubility of non-electrolytes (including polymers) in a given solvent. For a substance B,

$$\delta_{\mathrm{B}} = \left(\frac{\Delta_{\mathrm{vap}}E_{\mathrm{m,B}}}{V_{\mathrm{m,B}}}\right)^{1/2}$$

where $\Delta_{\mathrm{vap}}E_{\mathrm{m,B}}$ is the molar energy of vaporization at zero pressure and $V_{\mathrm{m,B}}$ is the molar volume.
Notes:

1. For a substance of low molecular weight, the value of the solubility parameter can be estimated most reliably from the enthalpy of vaporization and the molar volume.
2. The solubility of a substance B can be related to the square of the difference between the solubility parameters for supercooled liquid B and solvent at a given temperature, with appropriate allowances for entropy of mixing. Thus, a value can be estimated from the solubility of the solid in a series of solvents of known solubility parameter. For a polymer, it is usually taken to be the value of the solubility parameter of the solvent producing the solution with maximum intrinsic viscosity or maximum swelling of a network of the polymer. See J.H. Hildebrand, R.L.Scott, The Solubility of Nonelectrolytes, 3rd ed., Reinhold Publishing (1950); Dover Publications (1964), Chap. VII, p.129; Chap. XXIII, for the original definition, theory, and extensive examples.
3. The SI units are $\mathrm{Pa}^{1/2} = \mathrm{J}^{1/2}\,\mathrm{m}^{-3/2}$, but units used frequently are $(\mu\mathrm{Pa})^{1/2} = (\mathrm{J\ cm}^{-3})^{1/2}$ or $(\mathrm{cal\ cm}^{-3})^{1/2}$, where $1\ (\mathrm{J\ cm}^{-3})^{1/2} \approx 2.045\ (\mathrm{cal\ cm}^{-3})^{1/2}$. The unit calorie is discouraged as obsolete.

Source:
PAC, 2008, *80*, 233 *(Glossary of terms related to solubility (IUPAC Recommendations 2008))* on page 264

solubility product

The product of the ion activities raised to appropriate powers of an ionic solute in its saturated solution expressed with due reference to the dissociation equilibria involved and the ions present.

Source:
Orange Book, p. 83

solute

The minor component of a solution which is regarded as having been dissolved by the solvent.

Source:
Orange Book, p. 83

solute-volatilization interference

in flame spectroscopy

Interference due to changes in the volatilization rate of the dry aerosol particles in the case when volatilization of the analyte is incomplete in the presence and/or absence of the concomitant. This interference can either be specific, if the analyte and interferent form a new phase of different thermostability, as when Mg and Al form $MgAl_2O_4$ in an air–acetylene flame, or non-specific, if the analyte is simply dispersed in a large excess of the interferent, as when Ag is dispersed in ThO_2. If the interferent has a high boiling point, this latter is sometimes referred to as a blocking interference. It is often difficult to make sharp distinctions between the specific and non-specific solute-volatilization interferences.

Source:
Orange Book, p. 136

solution

Also contains definition of: solvent

A liquid or solid phase containing more than one substance, when for convenience one (or more) substance, which is called the solvent, is treated differently from the other substances, which are called solutes. When, as is often but not necessarily the case, the sum of the mole fractions of solutes is small compared with unity, the solution is called a dilute solution. A superscript attached to the ∞ symbol for a property of a solution denotes the property in the limit of infinite dilution.

Source:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 535
Orange Book, p. 83
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2214

solvation

Any stabilizing interaction of a solute (or solute moiety) and the solvent or a similar interaction of solvent with groups of an insoluble material (i.e. the ionic groups of an ion-exchange resin). Such interactions generally involve electrostatic forces and van der Waals forces, as well as chemically more specific effects such as hydrogen bond formation.

See also: cybotactic region

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1164

solvation energy

The change in Gibbs energy when an ion or molecule is transferred from a vacuum (or the gas phase) to a solvent. The main contributions to the solvation energy come from:

1. the cavitation energy of formation of the hole which preserves the dissolved species in the solvent;
2. the orientation energy of partial orientation of the dipoles;
3. the isotropic interaction energy of electrostatic and dispersion origin; and
4. the anisotropic energy of specific interactions, *e.g.* hydrogen bonds, donor-acceptor interactions *etc.*

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1962

solvatochromic relationship

A linear free-energy relationship based on solvatochromism.
See also: Kamlet–Taft solvent parameters

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1164

solvatochromism

The (pronounced) change in position and sometimes intensity of an electronic absorption or emission band, accompanying a change in the polarity of the medium. Negative (positive) solvatochromism corresponds to a hypsochromic (bathochromic) shift with increasing solvent polarity.
See also: Dimroth–Reichardt E_T parameter, Z-value

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1164
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2274

solvent extraction

The process of transferring a substance from any matrix to an appropriate liquid phase. If the substance is initially present as a solute in an immiscible liquid phase the process is synonymous with liquid-liquid extraction.
Notes:

1. If the extractable material is present in a solid (such as a crushed mineral or an ore) the term leaching may be more appropriate. The extractable material may also be a liquid entrapped within or adsorbed on a solid phase.
2. Common usage has established this term as a synonym for liquid-liquid distribution. This is acceptable provided that no danger of confusion with extraction from solid phases exists in a given context.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2379

solvent front

in chromatography

The front line of the eluent.

Source:
Orange Book, p. 99

solvent

in liquid-liquid distribution

The term applied to the whole initial liquid phase containing the extractant.
Notes:

1. The solvent may contain only one extractant or it may be a composite homogeneous mixture of extractant(s) with diluent(s) and also sometimes modifiers and accelerators.
2. The term solvent must not be used as a synonym for any of the individual components of a composite liquid phase even where, in the case of a single component (e.g. 3-methylbutan-2-one or tributyl phosphate), it becomes identical with the extractant.
3. The term may be qualified to denote the extract from a given processing step e.g. loaded solvent.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2381

solvent ion exchange (SIX) [obsolete]

This term is not recommended.
See: liquid ion exchange

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2379

solvent isotope effect

A kinetic or equilibrium isotope effect resulting from change in the isotopic composition of the solvent.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1130

solvent migration-distance

in chromatography

The distance travelled by the solvent front.

Source:
Orange Book, p. 99

solvent parameter

Quantitative measures of the capability of solvents for interaction with solutes. Such parameters have been based on numerous different physicochemical quantities, e.g. rate constants, solvatochromic shifts in ultraviolet/visible spectra, solvent-induced shifts in infrared frequencies, etc. Some solvent parameters are purely empirical in nature, i.e. they are based directly on some experimental measurement. It may be possible to interpret such a parameter as measuring some particular aspect of solvent–solute interaction or it may be regarded simply as a measure of solvent *polarity*. Other solvent parameters are based on analysing experimental results. Such a parameter is considered to quantify some particular aspect of solvent capability for interaction with solutes.
See also: Dimroth–Reichardt E_T parameter, Grunwald–Winstein equation, Kamlet–Taft solvent parameters, Koppel–Palm solvent parameters, solvophobicity parameter, Z-value

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1164

solvent regeneration

in extraction processes

Treatment of the solvent for re-cycling, e.g. by removal of degradation products or non-strippable solutes. The term solvent purification is synonymous, but the terms scrubbing, stripping and washing should not be used in this context.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2389

solvent shift

A shift in the frequency of a spectral band of a chemical species arising from interaction with its solvent environment.
See: bathochromic shift, hyposchromic shift

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2274

solvent-induced symmetry breaking

Breaking of symmetry of a molecular species by interactions with the solvent that can modify the molecular charge distribution, to favour asymmetrical configurations.
Note:
An example is the stabilization by a polar solvent of a light-induced charge transfer state in a symmetric donor–acceptor–donor system.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 422

solvolysis

Also contains definition of: alcoholysis

Generally, reaction with a solvent, or with a lyonium ion or lyate ion involving the rupture of one or more bonds in the reacting solute. More specifically the term is used for substitution elimination and fragmentation reactions in which a solvent species is the nucleophile ('alcoholysis' if the solvent is an alcohol, etc.).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1165

solvophobicity parameter, *Sp*

A solvent parameter defined by:

$$Sp = 1 - \frac{M}{M(\text{ hexadecane })}$$

derived from the Gibbs energy of transfer ($\Delta_\mathrm{t} G^\circ$) of a series of solutes from water to numerous aqueous-organic mixtures and to pure solvents:

$$\Delta_\mathrm{t} G^\circ(\text{ to solvent }) = M\,R_\mathrm{T} + D$$

where R_T is a solute parameter, and M and D characterize the solvent. The M values are used to define a solvent solvophobic effect so that S_p values are scaled from unity (water) to zero (hexadecane).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1165

solvus

A line on a binary phase diagram (or a surface on a ternary phase diagram) that defines the limit of solid solubility under equilibrium conditions.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 590

SOMO

A Singly Occupied Molecular Orbital (such as the half-filled HOMO of a radical).
See also: frontier orbitals

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1165

sonication

Irradiation with (often ultra)sound waves, e.g. to increase the rate of a reaction or to prepare vesicles in mixtures of surfactants and water.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1165

sonogel

Colloidal gel produced by the action of ultrasonically induced cavitation.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1808

sonoluminescence

Luminescence induced by sound waves.
See: triboluminescence

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2274

sonosol

Sol produced by the action of ultrasonically induced cavitation.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1806

soot

A randomly formed particulate carbon material and may be coarse, fine and/or colloidal in proportions depending on its origin. Soot consists of variable quantities of carbonaceous and inorganic solids together with absorbed and occluded tars and resins.
Note:
An unwanted by-product of incomplete combustion or pyrolysis. Soot generated within flames consists essentially of aggregates of spheres of carbon. Soot found in domestic fireplace chimneys contains few aggregates but may contain substantial amounts of particulate fragments of coke or char. Soot from diesel engines consists essentially of aggregates together with tars and resins. For historical reasons, the term soot is sometimes incorrectly used for carbon black. This misleading use should be avoided.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 504

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2215

Soret band

A very strong absorption band in the blue region of the optical absorption spectrum of a haem protein.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1298

sorption

in colloid chemistry

The process by which a substance (sorbate) is sorbed (adsorbed or absorbed) on or in another substance (sorbent).
See also: absorption, adsorption, desorption

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2215
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 584

See also:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 854

sorption isotherm

in ion exchange

The concentration of a sorbed species in the ion exchanger, expressed as a function of its concentration in the external solution under specified conditions and at constant temperature.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 854

sorption techniques

in trace analysis

Techniques based on the distribution of components being separated between two phases, one of which is stationary and the other mobile. The advantage of some chromatographic methods is the possibility of combining the preconcentration and determination steps, as well as improving the speed of determination, and the possibility of separation of components with similar properties, and of achieving high values of the preconcentration coefficient. The methods enable analyses of microamounts of substances. Ion-exchange chromatography is not widely used owing to the great volumes of solutions being treated and, consequently, to a great degree to the variation in the blank, and to some diffusional limitations. Static ion-exchange, which is much simpler and more readily carried out, is practised quite widely.

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1199

sorptive insertion

in surface catalysis

This is analogous to the process of ligand insertion in coordination chemistry.

$$H^{*} + C_2H_4(g) \longrightarrow {}^{*}C_2H_5$$

This reaction might also be imagined to proceed by adsorption of C_2H_4 followed by ligand migration (an associative surface reaction).

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 84

sp

See: torsion angle

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

space charge

in a semiconductor

At the surface region of a semiconductor the surface excess or deficiency of electrons constitutes a space charge.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 443

space formula

Synonymous with stereochemical formula.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

space time

in catalysis

The reciprocal of space velocity.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 82

space velocity

in catalysis

Defined as v_m, v_v, and v_a where the v_is represent the rate of feed of the given reactant fed per unit mass, volume or surface area of the catalyst.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 82

spacer

A flexible segment used to link successive mesogenic units in the molecules of MCPLCs (main-chain polymer liquid crystals) or to attach mesogenic units as side-groups onto the polymer backbone of SGPLCs (side-group polymer liquid crystals).

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 504

spark (source) ionization

in mass spectrometry

Occurs when a solid sample is vaporized and partially ionized by an intermittent discharge. It is recommended that the word 'source' be dropped from this term.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548
Orange Book, p. 204

spatial-distribution interference

in flame spectroscopy

Interference which may occur when changes in concentration of concomitants affect the mass flow rates or mass flow patterns of the analyte species in the flame. If they are caused by changes in volume and rise velocity of the gases formed by combustion, in extreme cases manifesting themselves by changes in the size and/or shape of the flame, they are non-specific and are called flame-geometry interferences.

Source:
Orange Book, p. 171

spatially resolving detector

of radiation

A detector for the measurement of the spatial distribution of the radiation. Spatially resolving detectors can be divided into two groups:

1. the photosensitive area consists of a matrix of discrete photosensitive elements, the pixels (picture elements) forming an array with the facility to separately read out the information, simultaneously or sequentially.
2. the photosensitive area consists of a single photosensitive element that must be scanned (e.g. image dissection tube.)

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1755

special salt effect

The initial steep rate increase observed in the kinetic electrolyte effect on certain solvolysis reactions, upon addition of some non-common ion salts, especially $LiClO_4$.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1165

speciation analysis

in chemistry

Analytical activities of identifying and/or measuring the quantities of one or more individual chemical species in a sample.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1070

speciation

in chemistry

Distribution of an element amongst defined chemical species in a system.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1070
This definition replaces an earlier definition of speciation.

species (taxonomic)

A taxonomic subdivision of a genus; a group of closely related, morphologically and physiologically similar individuals.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 166

specific

Attribute to a physical quantity obtained by division by mass. Specific volume is the volume of a sample divided by its mass.

Source:
Green Book, 2nd ed., p. 7

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 992

specific acid–base catalysis

Catalysis by acids or bases in solution is said to be specific when the only observable catalytic effects are those due to the ions formed from the solvent itself (e.g. if when water is the solvent the only observable catalysis is that due to the H^+ and OH^- ions).
See: general acid catalysis, general base catalysis

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 150

specific activity, *a*

in radiochemistry

For a specified isotope, or mixture of isotopes, the activity of a material divided by the mass of the material.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2515
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 993

specific adsorption

Ions become specifically adsorbed when short-range interactions between them and the interphase become important. They are believed then to penetrate into the inner layer and may (but not necessarily) come into contact with the surface. They are usually assumed to form a partial or complete monolayer.
See: non-specific adsorption

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 448

specific burn-up

The total energy released through induced nuclear transformations divided by the mass of a nuclear fuel.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1537

specific catalysis

The acceleration of a reaction by a unique catalyst, rather than by a family of related substances. The term is most commonly used in connection with specific hydrogen-ion or hydroxide-ion (lyonium ion or lyate ion) catalysis.
See also: general acid catalysis, general base catalysis, pseudo-catalysis

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1165

specific conductance

See: conductivity

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 993
Green Book, 2nd ed., p. 15

specific detector

in chromatography

A detector which responds to a single sample component or to a limited number of components having similar chemical characteristics.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 849

specific gravity

See: relative density

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2215
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2472

specific heat capacity, c

Heat capacity divided by mass.
See: heat capacity

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 993

specific

in analysis

A term which expresses qualitatively the extent to which other substances interfere with the determination of a substance according to a given procedure. Specific is considered to be the ultimate of selective, meaning that no interferences are supposed to occur.

Source:
PAC, 1983, *55*, 553 *(Recommendations for the usage of selective, selectivity and related terms in analytical chemistry)* on page 555

specific ionization

in nuclear chemistry

The number of ion pairs formed per unit distance along the track of an ionizing particle passing through matter.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552

specific permeability

in chromatography

A term expressing the resistance of an empty tube or packed column to the flow of a fluid (the mobile phase).

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 833

specific pore volume

of a catalyst

The total internal void volume per unit mass of adsorbent.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

specific retention volume

in chromatography

See: retention volumes *in chromatography*

Source:
Orange Book, p. 103
Orange Book, p. 104

specific surface area

in surface chemistry

When the area of the interface between two phases is proportional to the mass of one of the phases (e.g. for a solid adsorbent, for an emulsion or for an aerosol), the specific surface area (a, s or preferably a_s) is defined as the surface area divided by the mass of the relevant phase.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 583
Green Book, 2nd ed., p. 63

specific volume, v

Volume of a substance divided by its mass. It is the reciprocal of mass density.
See: volume content

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 993

specific weight

See: mass density

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2471

specifically absorbing ion

Ions which possess a chemical affinity for the surface in addition to the Coulomb interaction, where chemical is a collective adjective, embracing all interactions other than purely Coulombic. Examples are van der Waals or hydrophobic bonding, pi-electron exchange and complex formation. Specifically adsorbing ions can adsorb on an initially uncharged surface and hence provide it with a charge. The term specifically adsorbed applies to the sorption of all other ions having an affinity to the surface in addition to the purely Coulombic contribution.
See also: indifferent adsorbing ion

Source:
PAC, 1991, *63*, 895 *(Nomenclature, symbols, definitions and measurements for electrified interfaces in aqueous dispersions of solids (Recommendations 1991))* on page 899

specifically labelled

An isotopically labelled compound is designated as specifically labelled when a unique isotopically substituted compound is formally added to the analogous isotopically unmodified compound. In such a case, both position(s) and number of each labelling nuclide are defined.

Source:
Blue Book, p. 514
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1891

specifically labelled tracer

A tracer in which the label is present in a specified position.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

specimen

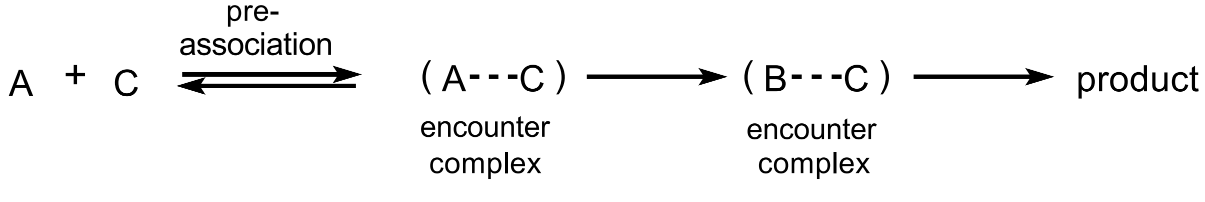
in analytical chemistry

A specifically selected portion of a material taken from a dynamic system and assumed to be representative of the parent material at the time it is taken. Although the specimen may not be reproducible in time, e.g. it may be taken from a flowing stream or a portion of blood, no separable sampling error exists since this error is unavoidably included with the corresponding error of the estimate of the property, function or analyte being studied. A specimen may be considered as a special type of sample, taken primarily in time rather than in space. The term 'specimen' has been used both as a representative unit and as a nonrepresentative (often better than most) unit of a population, usually in clinical, biological and mineralogical collections. 'Collections' in this case is used as either a noun or verb. This usage is almost always self-evident, and thus would not be confused with a time-type sample.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1202

spectator mechanism

A pre-association mechanism in which one of the molecular entities, **C**, is already present in an encounter pair with **A** during formation of **B** from **A**, but does not assist the formation of **B**, e.g.



The formation of **B** from **A** may itself be a bimolecular reaction with some other reagent. Since **C** does not assist the formation of **A**, it is described as being present as a spectator, and hence such a mechanism is sometimes referred to as a spectator mechanism.
See also: microscopic diffusion control

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1165

spectator-stripping reaction

An extreme type of stripping reaction in which one reaction product has almost the same direction and momentum as one of the reactant molecules had before the reactive collision occurred.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 186

spectral bandwidth error

in spectrochemical analysis

To measure the true shape, particularly the true maximum of an absorption band, the spectral bandwidth $\Delta\lambda$ of the instrument must be much less than the width of the absorption band. A spectral bandwidth error results from using too large a bandwidth relative to the absorption band being measured.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1456

spectral distribution

The variation of the spectral radiance with wavelength.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1453

spectral fluence rate, $E_{\lambda,\mathrm{o}}$

Derivative of fluence rate, E_o, with respect to wavelength, λ. SI unit is $\mathrm{W\ m^{-3}}$; common unit is $\mathrm{W\ m^{-2}\ nm^{-1}}$.
Note:
All spectral terms may also be defined as derivatives with respect to frequency, ν, or wavenumber, $\tilde{\nu}$, and are referred to, when necessary, as in terms of wavelength, or frequency or wavenumber, respectively.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 423

spectral intensity

See: spectral quantities

Source:
Green Book, 2nd ed., p. 31

spectral interference

in flame spectroscopy

Interference due to the incomplete isolation of the radiation emitted or absorbed by the analyte from other radiation detected by the instrument. Its occurrence may be established by comparing the measures of the analyte-free blank solution and the solvent blank.

Source:
Orange Book, p. 169

spectral irradiance, E_λ

Irradiance, E, at wavelength λ per unit wavelength interval. The SI unit is $\mathrm{W\ m^{-3}}$, but a commonly used unit is $\mathrm{W\ m^{-2}\ nm^{-1}}$.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2275

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2198

spectral overlap

In the context of radiative energy transfer, the integral, $J = \int_0^\infty f_\mathrm{D}'(\sigma)\ \varepsilon_\mathrm{A}(\sigma)\mathrm{d}\sigma$, which measures the overlap of the emission spectrum of the excited donor, D, and the absorption spectrum of the ground state acceptor, A; f_D' is the measured normalized emission of D, $f_\mathrm{D}' = \frac{f_\mathrm{D}(\sigma)}{\int_0^\infty f_\mathrm{D}(\sigma)\mathrm{d}\sigma}$, $f_\mathrm{D}(\sigma)$ is the photon exitance of the donor at wavenumber σ, and $\varepsilon_\mathrm{A}(\sigma)$ is the decadic molar absorption coefficient of A at wavenumber σ. In the context of Förster excitation transfer, J is given by:

$$J = \int_0^\infty \frac{f_\mathrm{D}'(\sigma)\ \varepsilon_\mathrm{A}(\sigma)}{\sigma^4}\mathrm{d}\sigma$$

In the context of Dexter excitation transfer, J is given by:

$$J = \int_{0}^{\infty} f_{\mathrm{D}}(\sigma)\, \varepsilon_{\mathrm{A}}(\sigma) \mathrm{d}\sigma$$

In this case f_{D} and ε_{A}, the emission spectrum of donor and absorption spectrum of acceptor, respectively, are both normalized to unity, so that the rate constant for energy transfer, k_{ET}, is independent of the oscillator strength of both transitions (contrast to Förster mechanism).
See: energy transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2275

spectral (photon) effectiveness

The reciprocal of the photon fluence rate, E_{p}^{0}, at wavelength λ, causing identical photoresponse, $\Delta \mathrm{y}$, per unit time ($\frac{\Delta \mathrm{y}}{\Delta t}$). The effectiveness spectrum is directly proportional to the conversion spectrum of the sensory pigment, if spectral attenuance is negligible.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2275

spectral photon exitance, $M_{\mathrm{p}\lambda}$

The photon exitance, M_{p}, at wavelength per unit wavelength interval. The SI unit is $\mathrm{s}^{-1}\ \mathrm{m}^{-3}$, but a commonly used unit is $\mathrm{s}^{-1}\ \mathrm{m}^{-2}\ \mathrm{nm}^{-1}$. Alternatively, the term can be used with the amount of photons (mol or its equivalent einstein) the SI unit then being $\mathrm{mol\ s}^{-1}\ \mathrm{m}^{-3}$ and the common unit $\mathrm{mol\ s}^{-1}\ \mathrm{m}^{-2}\ \mathrm{nm}^{-1}$.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2275

spectral photon flow, $\Phi_{\mathrm{p}\lambda}$

The photon flow, Φ_{p}, at wavelength λ per unit wavelength interval. The SI unit is $\mathrm{s}^{-1}\ \mathrm{m}^{-1}$, but a commonly used unit is $\mathrm{s}^{-1}\ \mathrm{nm}^{-1}$. Alternatively, the term can be used with the amount of photons (mol or its equivalent einstein), the SI unit then being $\mathrm{mol\ s}^{-1}\ \mathrm{m}^{-1}$ and the common unit $\mathrm{mol\ s}^{-1}\ \mathrm{nm}^{-1}$.

Source:
PAC, 1996, *68*, 2223 ***(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))*** on page 2275

spectral photon flux (photon irradiance), $E_{\mathrm{p}\lambda}$

The photon irradiance E_{p}, at wavelength λ per unit wavelength interval. The SI unit is $\mathrm{s^{-1}\ m^{-3}}$, but a commonly used unit is $\mathrm{s^{-1}\ m^{-2}\ nm^{-1}}$. Alternatively, the term can be used with the amount of photons (mol or its equivalent einstein), the SI unit then being $\mathrm{mol\ s^{-1}\ m^{-3}}$ and the common unit $\mathrm{mol\ s^{-1}\ m^{-2}\ nm^{-1}}$.

Source:
PAC, 1996, *68*, 2223 ***(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))*** on page 2275

spectral photon radiance, $L_{\mathrm{p}\lambda}$

The photon radiance, L_{p}, at wavelength per unit wavelength interval. The SI unit is $\mathrm{s^{-1}\ m^{-3}\ sr^{-1}}$, but a commonly used unit is $\mathrm{s^{-1}\ m^{-2}\ sr^{-1}\ nm^{-1}}$. Alternatively, the term can be used with the amount of photons (mol or its equivalent einstein) the SI unit then being $\mathrm{mol\ s^{-1}\ m^{-3}\ sr^{-1}}$ and the common unit $\mathrm{mol\ s^{-1}\ m^{-2}\ sr^{-1}\ nm^{-1}}$.

Source:
PAC, 1996, *68*, 2223 ***(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))*** on page 2276

spectral quantities

Quantities characterizing electromagnetic radiation (radiant power, energy, energy density, intensity, exitance, radiance, irradiance, etc.) derived by differentiation with respect to wavelength, frequency or wavenumber, e.g. spectral (concentration of) irradiance is the derivative of the irradiance with respect to wavelength (E_{λ}), frequency (E_{ν}) or wavenumber ($E_{\tilde{\nu}}$).

Source:
Green Book, 2nd ed., p. 31

spectral radiance, L_{λ}

Th e radiance, L, at wavelength λ per unit wavelength interval. The SI unit is $\mathrm{W\ m^{-3}\ sr^{-1}}$, but a commonly used unit is $\mathrm{W\ m^{-2}\ sr^{-1}\ nm^{-1}}$.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276

spectral radiant energy, Q_λ

Derivative of radiant energy, Q, with respect to wavelength λ. SI unit is $\mathrm{J\ m^{-1}}$; common unit is $\mathrm{J\ nm^{-1}}$.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 425

spectral radiant exitance, M_λ

The radiant exitance, M, at wavelength λ per unit wavelength interval. The SI unit is $\mathrm{W\ m^{-3}}$, but a commonly used unit is $\mathrm{W\ m^{-2}\ nm^{-1}}$.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276

spectral radiant flux

Synonymous with spectral radiant power.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276

spectral radiant intensity, I_λ

The radiation intensity, I at wavelength λ per unit wavelength interval. The SI unit is $\mathrm{W\ m^{-1}\ sr^{-1}}$, but a commonly used unit is $\mathrm{W\ nm^{-1}\ sr^{-1}}$.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276

spectral radiant power, P_λ

The radiant power at wavelength λ per unit wavelength interval. The SI unit is $\mathrm{W\ m^{-1}}$, but a commonly used unit is $\mathrm{W\ nm^{-1}}$.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276

See also:
PAC, 1985, *57*, 105 *(Names, symbols, definitions and units of quantities in optical spectroscopy (Recommendations 1984))* on page 112

spectral responsivity

The spectral output quantity of a system such as a photomultiplier, diode array, photoimaging device, or biological unit divided by the spectral irradiance $s(\lambda) = \frac{\mathrm{d}y(\lambda)}{\mathrm{d}E(\lambda)}$, simplified expression: $s(\lambda) = \frac{Y_\lambda}{E_\lambda}$, where Y_λ is the magnitude of the output signal for irradiation at wavelength λ and E_λ is the spectral irradiance of the parallel and perpendicular incident beam at the same wavelength.
See also: responsivity

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1749

spectral sensitivity, $S(\lambda)$

Referred to actinometers based on spectrophotometric measurements, $S_{\mathrm{ac}}(\lambda) = \Phi(\lambda)\ \varepsilon(\lambda_{\mathrm{obs}}) = \text{sensitivity or actinometric factor}$. $\Phi(\lambda)$ is the quantum yield of the actinometer at the excitation wavelength and λ_{obs} is the observation wavelength, which may be the same as or differ from the former.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 426

spectral sensitization

The process of increasing the spectral responsivity of a (photoimaging) system in a given wavelength region.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276

spectral spheradiance

Alternative term suggested for actinic flux.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2215

spectrochemical buffer

in atomic spectroscopy

Buffer added to samples and reference samples with the intention of making the measure of the analytical element less sensitive to changes in concentration of an interferent.

Source:
Orange Book, p. 159

spectrochemical carrier

in atomic spectroscopy

An additive which gives rise to a gas which can help to transport the vapour of the sample material into the excitation region of the source, e.g. carbon in an air atmosphere when carbon dioxide is formed.

Source:
Orange Book, p. 160

spectrogram

A spectrum as recorded by a spectrometer.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552

spectrograph

A combination of a spectral apparatus and a camera, which enables an image of a spectrum to be recorded. Spectra are recorded by a photographic emulsion or other means, e.g. two-dimensional electronic image sensors.

Source:
PAC, 1995, *67*, 1725 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-IX. Instrumentation for the spectral dispersion and isolation of optical radiation (IUPAC Recommendations 1995))* on page 1729

spectrometer

A general term for describing a combination of spectral apparatus with one or more detectors to measure the intensity of one or more spectral bands.
See also: sequential spectrometer, simultaneous spectrometer, multiplex spectrometer, filter spectrometer

Source:
PAC, 1995, *67*, 1725 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-IX. Instrumentation for the spectral dispersion and isolation of optical radiation (IUPAC Recommendations 1995))* on page 1729

spectroscope

A device which enables visual observation and evaluation of optical spectra (usually confined to the visible spectral region).

Source:
PAC, 1995, *67*, 1725 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-IX. Instrumentation for the spectral dispersion and isolation of optical radiation (IUPAC Recommendations 1995))* on page 1729

spectroscopy

Also contains definition of: spectrometry

The study of physical systems by the electromagnetic radiation with which they interact or that thay produce. Spectrometry is the measurement of such radiations as a means of obtaining information about the systems and their components. In certain types of optical spectroscopy, the radiation originates from an external source and is modified by the system, whereas in other types, the radiation originates within the system itself.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1738

spectrum analysis

The interpretation of the information present in an energy spectrum in terms of radiation energy and intensity.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552

specular reflectance (reflection factor), ρ

in optical spectroscopy

Radiant power specularly reflected from the surface of a system, P_{refl}, divided by the incident power, P_0:

$$\rho = \frac{P_{\text{refl}}}{P_0}$$

Source:
PAC, 1985, *57*, 105 *(Names, symbols, definitions and units of quantities in optical spectroscopy (Recommendations 1984))* on page 115

speed, v, c

Scalar quantity equal to the absolute value of the velocity vector.

Source:
Green Book, 2nd ed., p. 11
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 993

speed distribution function, $F(c)$

Probability density of finding a particle with speed within an interval between c and $c + \mathrm{d}c$.

Source:
Green Book, 2nd ed., p. 39

speed of light in a vacuum

Universal fundamental physical constant representing the speed of electromagnetic waves in vacuum; by definition c_0 is exactly = $299\ 792\ 458\ \mathrm{m\ s^{-1}}$.

Source:
CODATA Bull. 1986, *63*, 1

spherical carbonaceous mesophase

A term which describes the morphology of carbonaceous mesophase which is formed in the isotropic pitch matrix. The spherical carbonaceous mesophase usually has a lamellar structure consisting of flat aromatic molecules arranged in parallel layers which are perpendicular to the sphere/isotropic phase interface. On coalescence, this spherical mesophase loses its characteristic morphology and is converted to the bulk mesophase.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 505

spherical radiance

Same as radiant exitance, M. It is the integration of the radiant power, P, leaving a source over the solid angle and over the whole wavelength range.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276

spherical radiant exposure

Synonymous with fluence.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276

spherulite

A polycrystalline, roughly spherical morphology consisting of lath, fibrous or lamellar crystals emanating from a common centre. Space filling is achieved by branching, bending or both, of the constituent fibres or lamellae.

Source:
Purple Book, p. 83

spin conservation rule (Wigner rule)

For both radiative and radiationless transitions, the principle that transitions between terms of the same multiplicity are spin-allowed, while transitions between terms of different multiplicity are spin-forbidden.

Source:
Orange Book, p. 185
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2277
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 234

spin contamination

In unrestricted Hartree–Fock method, the wavefunctions obtained are eigenfunctions of the Hamiltonian and the spin projection $\boldsymbol{S}_z$ operators, but not eigenfunctions of the $\boldsymbol{S}^2$ operator. As a result, the wavefunctions of the doublet systems are spin-contaminated to some extent by admixtures of quartet, sextet, and higher spin states. The eigenvalues of the $\boldsymbol{S}^2$ operator are given as a measure of the spin contamination.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1962

spin crossover

A type of molecular magnetism that is the result of electronic instability (see electronic stability) caused by external constraints (temperature, pressure, or electromagnetic radiation), which induce structural changes at molecular and lattice levels. The phenomenon is most characteristic of first-row transition metal complexes, *e g,.* those of Fe^{II}. An example of spin-crossover complexes (the term of spin-state isomers is also used) is $[Fe(2\text{-pic})_3]Cl_2{\cdot}EtOH$ (2-pic = 2-picolylamine). At the Fe–N distance of $203.2\ \text{pm}$ ($115\ \text{K}$), the complex has an electronic low-spin state ($^1A_1$), whereas stretching the bond up to $219.9\ \text{pm}$ at $227\ \text{K}$ induces the transition to a high-spin state ($^5T_2$).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1963

spin density

The unpaired electron density at a position of interest, usually at carbon, in a radical It is often measured experimentally by electron paramagnetic resonance [EPR, ESR (electron spin resonance)] spectroscopy through hyperfine coupling constants of the atom or an attached hydrogen.
See also: radical centre

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1166

spin label

Also contains definition of: spin probe

A stable paramagnetic group (typically a nitryl radical) that is attached to a part of a molecular entity whose microscopic environment is of interest and may be revealed by the electron spin resonance (ESR) spectrum of the spin label. When a simple paramagnetic molecular entity is used in this way without covalent attachment to the molecular entity of interest it is frequently referred to as a 'spin probe'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1166

spin polarization

Static and dynamic spin polarization effects are distinguished. The static polarization of an electron spin occurs in the C–H bonds of aromatic radicals where the σ-electron closest to an unpaired π-electron tends to have its spin parallel to that of the π-electron. Likewise, static spin polarization arises in the π-system of conjugated radicals: the electron of the doubly occupied molecular orbital prefers to take a closer spatial position to the odd one, which spin is parallel to the latter. The effect reflects the energy unfavourable situation if an electron of opposite spin were to come nearby.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1963

spin projection

A component, M_S, of the angular spin moment $\boldsymbol{S}$ along an arbitrary axis (usually chosen as the z-direction). M_S can take the values between $-S$ and S: $-S$, $-S+1$,..., $S-1$, S. The term is also used to denote an operation (spin-symmetry projection) allowing one to eliminate spin contamination in the cases where wavefunctions are not eigenfunctions of the operator $\boldsymbol{S}^2$.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1963

spin trapping

Also contains definitions of: spin adduct, spin counting

In certain reactions in solution a transient radical will interact with a diamagnetic reagent to form a more persistent radical. The product radical accumulates to a concentration where detection and, frequently, identification are possible by EPR/ESR spectroscopy. The key reaction is usually one of attachment; the diamagnetic reagent is said to be a 'spin trap' and the persistent product radical is then the 'spin adduct'. The procedure is referred to as spin trapping, and is used for monitoring reactions involving the intermediacy of reactive radicals at concentrations too low for direct observation. Typical spin traps are *C*-nitroso compounds and nitrones, to which reactive radicals will rapidly add to form nitryl radicals. A quantitative development, in which essentially all reactive radicals generated in a particular system are intercepted, has been referred to as 'spin counting'. Spin trapping has also been adapted to the interception of radicals generated in both gaseous and solid phases. In these cases the spin adduct is in practice transferred to a liquid solution for observation in order to facilitate interpretation of the EPR/ESR spectra of the radicals obtained.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1166

spin-allowed electronic transition

An electronic transition which does not involve a change in the spin part of the wavefunction.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2276

spin-flip method

Quantum mechanical method for the calculation of open-shell excited states. The method accurately describes low-lying multi-configurational electronic states of diradicals and triradicals in an efficient and robust single-reference scheme. The target low-spin states (e.g., S = 0 or S = 1/2) are described as spin-flipping excitations (S = −1) from a well-behaved high-spin reference state (e.g., S = 1 or S = 3/4). By employing theoretical models of increasing complexity for the reference (e.g., SCF, MP2, CCSD), the accuracy in the target states' description can be systematically improved. The SF methods result in multistate single-step computational schemes, e.g., several low-lying states can be computed in a single calculation that includes both dynamical and non-dynamical correlation effects.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 427

spin-flip transition

A rotation of electron spins, above a critical magnetic field, H_c, in an antiferromagnet from parallel to largely perpendicular alignment, relative to an applied magnetic field, H_a, for $H_a > H_c$.
See also: simultaneous pair transitions

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 590

spin-glass transition

A second-order transition from a paramagnetic or ferromagnetic state to a spin-glass state in which spins from moment-bearing solute atoms become ordered randomly in a non-magnetic host such that the net magnetization of any region is zero.
Examples: Au–Fe, Cu–Mn and Mo–Fe

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 591

spin-orbit coupling

The interaction of the electron spin magnetic moment with the magnetic moment due to the orbital motion of the electron. One consequence of spin-orbit coupling is the mixing of zero-order states of different multiplicity. This effect may result in fine structure called spin-orbit splitting.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2277

spin-orbit coupling constant, *A*

Coefficient in the spin-orbit coupling term in the hamiltonian.

Source:
Green Book, 2nd ed., p. 23

spin-orbit splitting

Removal of state degeneracy by spin-orbit coupling.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2277

spin-Peierls transition

A magneto-elastic transition that occurs in quasi one-dimensional antiferromagnetic materials when the magnetic free energy decrease due to the formation of singlet spin pairs outweighs the increase in lattice free energy occurring as a result of the dimerization of the regular array. Example: The transition in tetrathiafulvalenium bis(dithiolene)cuprate at $12\ \mathrm{K}$.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 591

spin-state transition

An electronic transition from a high-spin state to a low-spin state, or vice versa. Example: With an increase in temperature Co^{3+} ions in $\mathrm{LaCoO_3}$ transform from a low-spin state ($\mathrm{t}_{2g}^{6}\mathrm{e}_{g}^{0}$) to the high-spin state ($\mathrm{t}_{2g}^{4}\mathrm{e}_{g}^{2}$).

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 591

spin-statistical factor (in diffusion-controlled reactions)

From the possible encounter pairs between states of different spin multiplicity, only those conserving multiplicity in going to products are expected to react.
Note:
This factor determines the efficiency of diffusion-controlled reactions, which have an encounter-controlled rate. Typical examples are quenching of fluorescence of aromatic hydrocarbons by O_2 , quenching of triplet states by O_2 , and triplet–triplet annihilation.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 428

spinodal

Curve defining the region of composition and temperature for a binary mixture across which a transition occurs from conditions where single-phase mixtures are metastable to conditions where single-phase mixtures are unstable and undergo phase separation by spinodal decomposition.

Notes:

1. The spinodal curve for a binary mixture is defined as the geometrical locus of all states with

$$\left(\frac{\partial^2 \Delta_{\text{mix}} G}{\partial \phi^2}\right)_{T,p} = 0.$$

2. In the unstable region bounded by the spinodal curve, phase domain separation is spontaneous, *i.e.,* no nucleation step is required to initiate the separation process.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1998

spinodal decomposition

A clustering reaction in a homogeneous, supersaturated solution (solid or liquid) which is unstable against infinitesimal fluctuations in density or composition. The solution therefore separates spontaneously into two phases, starting with small fluctuations and proceeding with a decrease in the Gibbs energy without a nucleation barrier.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 591

spin–spin coupling

The interaction between the spin magnetic moments of different electrons and/or nuclei. It causes, e.g. the multiplet pattern in nuclear magnetic resonance spectra.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2277

spin–spin coupling constant, J_{AB}

Coefficient of the indirect spin–spin coupling between two nuclei (A and B) in a magnetic resonance hamiltonian.

Source:
Green Book, 2nd ed., p. 15

spiro chain

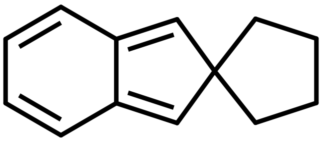
in a polymer

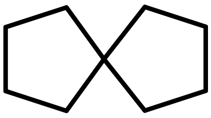
A double-strand chain consisting of an uninterrupted sequence of rings, with adjacent rings having only one atom in common. Alternatively, a spiro chain is a double-strand chain with adjacent constitutional units joined to each other through three atoms, two on one side and one on the other side of each constitutional unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2295

spiro compounds

Compounds having one atom (usually a quaternary carbon) as the only common member of two rings, e.g.





Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

spiro macromolecule

A double-strand macromolecule consisting of an uninterrupted sequence of rings, with adjacent rings having only one atom in common. Alternatively, a spiro macromolecule is a double-strand macromolecule with adjacent constitutional units joined to each other through three atoms, two on one side and one on the other side of each constitutional unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2295

spiro union

Also contains definitions of: free spiro union, spiro atom

A union formed by a single atom which is the only common member of two rings. The common atom is designated as the spiro atom. A free spiro union is one which constitutes the only union direct or indirect between the two rings.

Source:
Blue Book, p. 37

splicing

1. *of RNA*: The procedure by which introns are removed from eukaryotic precursor mRNA molecules and adjacent exon sequences are joined together (spliced).
2. *of DNA*: Manipulation for joining together double-stranded DNA fragments with protruding single-stranded 'sticky ends' by means of ligases.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 166

spontaneous emission

That mode of emission which occurs even in the absence of a perturbing external electromagnetic field. The transition between states, n and m, is governed by the Einstein coefficient of spontaneous emission, A_{nm}.
See also: stimulated emission

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2277

spontaneous fission

Nuclear fission which occurs without the addition of particles or energy to the nucleus

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

spot

in chromatography

A zone in paper and thin-layer chromatography of approximately circular appearance.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 834
Orange Book, p. 96

sprayer

in flame spectroscopy

The particular part of a nebulizer where the aspirated liquid is disrupted by the gas-jet into a spray.

Source:
Orange Book, p. 165

spread monolayer

It may happen that a component is virtually insoluble in both of two adjoining phases, but is present as a monolayer between them. Such a layer can be produced by spreading.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 591

spreading function

in chromatography

The normalized signal produced, as a function of elution volume at the outlet of a size-exclusion chromatography set-up, by an instantaneous injection of a uniform sample.

Source:
Purple Book, p. 69

spreading wetting

A process in which a drop of liquid spreads over a solid or liquid substrate.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 597

sputter yield

The number of particles sputtered from the surface of a target per primary ion.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

sputtering

Removal of surface material (atoms, clusters and molecules) by particle bombardment.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

square-wave current

In square-wave polarography, the component of the current that is associated with the presence of a substance B. This component may be either faradaic (if B is electroactive) or non-faradaic (if B is surface-active).

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1499

stability constant

An equilibrium constant that expresses the propensity of a substance to form from its component parts. The larger the stability constant, the more stable is the species. The stability constant (formation constant) is the reciprocal of the instability constant (dissociation constant).

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1298

stable

As applied to chemical species, the term expresses a thermodynamic property, which is quantitatively measured by relative molar standard Gibbs energies. A chemical species A is more stable than its isomer B if $\Delta_r G^\circ > 0$ for the (real or hypothetical) reaction

$$\mathrm{A} \rightarrow \mathrm{B},$$

under standard conditions. If for the two reactions:

$$\mathrm{P} \rightarrow \mathrm{X} + \mathrm{Y} \qquad (\Delta_r G_1^o)$$

$$\mathrm{Q} \rightarrow \mathrm{X} + \mathrm{Z} \qquad (\Delta_r G_2^o)$$

$\Delta_r G_1^o > \Delta_r G_2^o$, P is more stable relative to the product Y than is Q relative to Z. Both in qualitative and quantitative usage the term stable is therefore always used in reference to some explicitly stated or implicitly assumed standard. The term should not be used as a synonym for unreactive or 'less reactive' since this confuses thermodynamics and kinetics. A relatively more stable chemical species may be more reactive than some reference species towards a given reaction partner.
See also: inert, unstable

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1166

stable film, metastable film

A film often thins gradually to a thickness at which it either ruptures or converts abruptly to an equilibrium. Rupture under these conditions characterizes unstable films, whereas transition to an equilibrium film characterizes (meta)stable films.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 614

stable ion

in mass spectrometry

An ion which is not sufficiently excited to dissociate spontaneously into a daughter ion and associated neutral fragment(s) or to react further in any other way within the time scale of the experiment, e.g. until hitting the detector.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

staggered conformation

The conformation of groups attached to two adjacent atoms if the torsion angles are such that the groups are as far away as possible from an eclipsed arrangement.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

stagnant inversion

in atmospheric chemistry

See: temperature inversion

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2215

stand-by state

in analysis

The condition of an instrument where the analytical procedure can begin immediately.
See: shut-down state, start-up time

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1664

standard acceleration of free fall

Acceleration defined as $g_n = 9.806\ 65\ \mathrm{m\ s^{-2}}$.

Source:
CODATA Bull. 1986, *63*, 1

standard atmosphere

Pressure defined as $101\ 325\ \mathrm{Pa}$ and used as unit of pressure with the symbol atm.

Source:
CODATA Bull. 1986, *63*, 1
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 993

standard atomic weights

Recommended values of relative atomic masses of the elements revised biennially by the IUPAC Commission on Atomic Weights and Isotopic Abundances and applicable to elements in any normal sample with a high level of confidence. A normal sample is any reasonably possible source of the element or its compounds in commerce for industry and science and has not been subject to significant modification of isotopic composition within a geologically brief period.

Source:
Green Book, 2nd ed., p. 94

standard chemical potential

Of substance B at temperature T, $\mu_{\mathrm{B}}^{\mathrm{o}}(T)$, is the value of the chemical potential under specified standard conditions (in the standard state).

Source:
Green Book, 2nd ed., p. 53

See also:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 536

standard concentration

Chosen value of amount concentration denoted by $c^{\ominus}$ or c° and usually equal to $1\ \mathrm{mol\ dm^{-3}}$.
See also: standard molality

Source:
Green Book, 2nd ed., p. 54

standard conditions for gases

Temperature, $273.15\ \mathrm{K}$ (0 °C) and pressure of 10^5 pascals. IUPAC recommends that the former use of the pressure of 1 atm as standard pressure (equivalent to $1.01325 \times 10^5\ \mathrm{Pa}$) should be discontinued.
See: STP

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2216

standard deviation, *s*

The positive square root of the sum of the squares of the deviations between the observations and the mean of the series, divided by one less than the total number in the series. The standard deviation is the positive square root of the variance, a more fundamental statistical quantity.

Source:
Orange Book, p. 5

See also:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 599
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2216

standard electrode potential, E°

The value of the standard emf of a cell in which molecular hydrogen under standard pressure is oxidized to solvated protons at the left-hand electrode.

Source:
Green Book, 2nd ed., p. 59

standard electromotive force

Quantity defined by $E^{\circ} = -\frac{\Delta_{\mathrm{r}}G^{\circ}}{n\,F} = \frac{R\,T}{n\,F}\ln K^{\circ}$, where $\Delta_{\mathrm{r}}G^{\circ}$ is the standard Gibbs energy of the cell reaction in the direction in which reduction occurs at the right-hand electrode in the diagram representing the cell ('reduction at right'), K° is the standard equilibrium constant for this reaction, n its charge number, F the Faraday constant, R the gas constant and T the thermodynamic temperature.

Source:
Green Book, 2nd ed., p. 58

standard entropy of activation, $\Delta^{\ddagger}S^{\circ}$, $\Delta^{\ddagger}S$

Entropy change associated with the activation reaction.

See: standard reaction quantities

Source:
Green Book, 2nd ed., p. 57

standard equilibrium constant, K°, K

Synonym: thermodynamic equilibrium constant

Quantity defined by $K^\circ = \mathrm{e}^{-\Delta_r G^\circ / RT}$ where $\Delta_r G^\circ$ is the standard reaction Gibbs energy, R the gas constant and T the thermodynamic temperature. Some chemists prefer the name thermodynamic equilibrium constant and the symbol K.

Source:
Green Book, 2nd ed., p. 50

See also:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 548

standard Gibbs energy of activation $\Delta^{\ddagger} G^\circ$, $\Delta^{\ddagger} G$

Standard Gibbs energy change associated with the activation reaction
See: standard reaction quantities

Source:
Green Book, 2nd ed., p. 57

standard hydrogen electrode

For solutions in protic solvents, the universal reference electrode for which, under standard conditions, the standard electrode potential (H^+ / H_2) is zero at all temperatures. The absolute electrode potential of the hydrogen electrode under standard conditions can be expressed in terms of thermodynamic quantities by applying a suitable Born–Haber cycle, thus:

$$E^\circ(\mathrm{H}^+/\mathrm{H}_2)(\mathrm{abs}) = \Delta_{\mathrm{at}} G^\circ + \Delta_{\mathrm{ion}} G^\circ + \frac{\alpha^{\mathrm{o,S}}_{\mathrm{H}^+}}{F}$$

where $\Delta_{\mathrm{at}} G^\circ$ and $\Delta_{\mathrm{ion}} G^\circ$ are the atomization and ionization Gibbs energies of H_2, $\alpha^{\mathrm{o,S}}_{\mathrm{H}^+}$ is the real potential of H_2 in solvent S and F is the Faraday constant. The recommended absolute electrode potential of the hydrogen electrode is:

$$E^\circ(\mathrm{H}^+/\mathrm{H}_2)^{\mathrm{H_2O}}(\mathrm{abs}) = (4.44 \pm 0.02)\ \mathrm{V} \qquad \text{at} \quad 298.15\ \mathrm{K}$$

Source:
PAC, 1986, *58*, 955 *(The absolute electrode potential: an explanatory note (Recommendations 1986))* on page 957

standard molality $m^{\ominus}$, m°

Chosen value of molality and usually equal to $1\ \mathrm{mol\ kg^{-1}}$.

Source:
Green Book, 2nd ed., p. 54

See also:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 538

standard potential of an electrode reaction

Synonymous with standard electrode potential.

Source:
Green Book, 2nd ed., p. 59

standard potential of the reaction in a chemical cell

Synonymous with standard electromotive force.

Source:
Green Book, 2nd ed., p. 58

standard pressure

Chosen value of pressure denoted by $p^{\ominus}$ or p°. In 1982 IUPAC recommended the value $10^5\ \mathrm{Pa}$, but prior to 1982 the value $101\ 325\ \mathrm{Pa}\ (= 1\ \mathrm{atm})$ was usually used.

Source:
Green Book, 2nd ed., p. 54
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 536

standard reaction quantities

Infinitesimal changes in thermodynamic functions with extent of reaction divided by the infinitesimal increase in the extent when all the reactants and products are in their standard states. For the quantity X they should be denoted by $\Delta_r X^{\circ}$, but usually only ΔX° is used. For specific types of reactions the subscript r is replaced by: f for formation, c for combustion, a for atomization and superscript ‡ for activation.

Source:
Green Book, 2nd ed., p. 52

standard solution

Also contains definitions of: primary standard, secondary standard

A solution of accurately known concentration, prepared using standard substances in one of several ways. A primary standard is a substance of known high purity which may be dissolved in a known volume of solvent to give a primary standard solution. If stoichiometry is used to establish the strength of a titrant, it is called a secondary standard solution. The term secondary standard can also be applied to a substance whose active agent contents have been found by comparison against a primary standard. Concentrations of standard solutions may be expressed in kmol m^{-3}, mol dm^{-3}, or in terms more closely related to those used in specific titrations (as titres).

Source:
Orange Book, p. 48

standard state

State of a system chosen as standard for reference by convention. Three standard states are recognized: For a gas phase it is the (hypothetical) state of the pure substance in the gaseous phase at the standard pressure $p = p^{\circ}$, assuming ideal behaviour. For a pure phase, or a mixture, or a solvent in the liquid or solid state it is the state of the pure substance in the liquid or solid phase at the standard pressure $p = p^{\circ}$. For a solute in solution it is the (hypothetical) state of solute at the standard molality m°, standard pressure p° or standard concentration c° and exhibiting infinitely dilute solution behaviour. For a pure substance the concept of standard state applies to the substance in a well defined state of aggregation at a well defined but arbitrarily chosen standard pressure.

Source:
Green Book, 2nd ed., p. 53

standard subtraction method

in electroanalytical chemistry

A variation of the standard addition method. In this procedure changes in the potential resulting from the addition of a known amount of a species which reacts stoichiometrically with the ion of interest (e.g. a complexing agent) are employed to determine the original activity or concentration of the ion.

Source:
Orange Book, p. 171

standard thermodynamic quantities

Values of thermodynamic functions in the standard state characterized by a standard pressure, molality or amount concentration, but not by temperature. Standard quantities are denoted by adding the superscript $^{\ominus}$ or $^{\circ}$ to the symbol of the quantity.

Source:
Green Book, 2nd ed., p. 53

See also:
PAC, 1994, *66*, 533 *(Standard quantities in chemical thermodynamics. Fugacities, activities and equilibrium constants for pure and mixed phases (IUPAC Recommendations 1994))* on page 536

standard uncertainty

Uncertainty of measurement expressed as one standard deviation.

Source:
VIM

stannoxanes

Compounds having the structure $H_3S_n[OSnH_2]_nOSnH_3$. Thus tin analogues of siloxanes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

stannylenes

See: stannylidenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

stannylidenes

Carbene analogues having the structure R_2Sn:. The older synonymous term stannylenes is no longer recommended.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1366

star copolymer

A copolymer where chains having different constitutional or configurational features are linked through a central moiety.

Source:
PAC, 1985, *57*, 1427 *(Source-based nomenclature for copolymers (Recommendations 1985))* on page 1435

star macromolecule

Also contains definitions of: *n*-star macromolecule, regular star macromolecule, variegated star macromolecule

A macromolecule containing a single branch point from which linear chains (arms) emanate.
Notes:

1. A star macromolecule with *n* linear chains (arms) attached to the branch point is termed an *n*-star macromolecule, e.g. five-star macromolecule.
2. If the arms of a star macromolecule are identical with respect to constitution and degree of polymerization, the macromolecule is termed a regular star macromolecule.
3. If different arms of a star macromolecule are composed of different monomeric units, the macromolecule is termed a variegated star macromolecule.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2296

star polymer

A polymer composed of star macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2304

Stark effect

Synonym: electrochromic effect

The splitting or shift of spectral lines in an electric field. Also called electrochromic effect.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2277

start-up time

in analysis

The time interval between turn-on of the instrument and its stand-by state.
See: shut-down state, stand-by state

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1664

starting line

Also contains definition of: starting point *in chromatography*

in chromatography

The point or line on a chromatographic layer where the substance to be chromatographed is applied.

Source:
Orange Book, p. 77

state crossing

See: avoided crossing, surface crossing

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2277

state diagram

See: Jablonski diagram

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2277

state-to-state kinetics

A branch of chemical kinetics concerned with the dynamics of reactions in which the reactant species are in known quantum states, and in which the quantum states of the products are determined.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 186

static fields mass spectrometer

An instrument which can separate selected ion beams with fields which do not vary with time. The fields are generally both electric and magnetic.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546
Orange Book, p. 202

static pressure

The pressure of a fluid at rest or in motion exerted perpendicularly to the direction of flow.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2208

static stability

In meteorology, the stability of the atmosphere in the vertical direction to vertical displacements. If Γ is the dry adiabatic lapse rate, dry air is stable if the lapse rate $-\frac{\mathrm{d}T}{\mathrm{d}z} < \Gamma$, unstable if $-\frac{\mathrm{d}T}{\mathrm{d}z} > \Gamma$ and neutral $-\frac{\mathrm{d}T}{\mathrm{d}z} = \Gamma$.
See: lapse rate, inversion

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2215

stationary phase (fermentation)

The phase of a culture of microorganisms or animal and plant cells cultured *in vitro* that follows the exponential growth phase and in which there is little or no growth. In some cases it is a phase of product formation, e.g. formation of secondary metabolites.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 166

stationary phase

in chromatography

One of the two phases forming a chromatographic system. It may be a solid, a gel or a liquid. If a liquid, it may be distributed on a solid. This solid may or may not contribute to the separation process. The liquid may also be chemically bonded to the solid (bonded phase) or immobilized onto it (immobilized phase). The expression chromatographic bed or sorbent may be used as a general term to denote any of the different forms in which the stationary phase is used. Particularly in gas chromatography where the stationary phase is most often a liquid, the term liquid phase is used for it as compared to the gas phase, i.e. the mobile phase. However, particularly in the early development of liquid chromatography, the term 'liquid phase' had also been used to characterize the mobile phase as compared to the 'solid phase' i.e. the stationary phase. Due to this ambiguity, the use of the term 'liquid phase' is discouraged. If the physical state of the stationary phase is to be expressed, the use of the adjective forms such as liquid stationary phase and solid stationary phase, bonded phase or immobilized phase is proposed.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 823

See also:
Orange Book, p. 98

stationary phase volume, V_s

in chromatography

The volume of the liquid stationary phase or the active solid in the column. The volume of any solid support is not included. In the case of partition chromatography with a liquid stationary phase, it is identical to the liquid phase volume.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 833

stationary state

1. (*in quantum mechanics*) : A state that does not evolve with time.
2. (*in kinetics*) :
   See: steady state

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1166

stationary-phase fraction

The volume of the stationary phase per unit volume of a packed column.

Source:
Orange Book, p. 100

statistical copolymer

A copolymer consisting of macromolecules in which the sequential distribution of the monomeric units obeys known statistical laws.
Note:
An example of a statistical copolymer is one consisting of macromolecules in which the sequential distribution of monomeric units follows Markovian statistics.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2301

statistical copolymerization

A copolymerization in which a statistical copolymer is formed.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2307

statistical segment

in polymers

A segment of an actual polymer chain which behaves, with respect to some property, virtually as a segment of a freely jointed chain.

Source:
Purple Book, p. 50

steady state

in liquid-liquid distribution

The state of a continuous process when it is operating in such a way that the concentration of solutes in exit streams remains constant with respect to time for constant feed concentrations, even though the two phases are not necessarily in thermodynamic equilibrium in any part of the process. The term equilibrium should not be used to describe this situation.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2390

steady state (stationary state)

Also contains definition of: steady state approximation (treatment)

1. In a kinetic analysis of a complex reaction involving unstable intermediates in low concentration, the rate of change of each such intermediate is set equal to zero, so that the rate equation can be expressed as a function of the concentrations of chemical species present in macroscopic amounts. For example, assume that **X** is an unstable intermediate in the reaction sequence:

$$\mathrm{A} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{X}$$

$$\mathrm{X} + \mathrm{C} \xrightarrow{k_2} \mathrm{D}$$

Conservation of mass requires that:

$$[\mathrm{A}] + [\mathrm{X}] + [\mathrm{D}] = [\mathrm{A}]_0$$

which, since $[\mathrm{A}]_0$ is constant, implies:

$$-\frac{\mathrm{d}\,[\mathrm{X}]}{\mathrm{d}t} = \frac{\mathrm{d}\,[\mathrm{A}]}{\mathrm{d}t} + \frac{\mathrm{d}\,[\mathrm{D}]}{\mathrm{d}t}.$$

Since $[\mathrm{X}]$ is negligibly small, the rate of formation of **D** is essentially equal to the rate of disappearance of **A**, and the rate of change of $[\mathrm{X}]$ can be set equal to zero. Applying the steady state approximation ($\frac{\mathrm{d}\,[\mathrm{X}]}{\mathrm{d}t} = 0$) allows the elimination of $[\mathrm{X}]$ from the kinetic equations, whereupon the rate of reaction is expressed:

$$\frac{\mathrm{d}\,[\mathrm{D}]}{\mathrm{d}t} = -\frac{\mathrm{d}\,[\mathrm{A}]}{\mathrm{d}t} = \frac{k_1\,k_2\,[\mathrm{A}]\,[\mathrm{C}]}{k_{-1} + k_2\,[\mathrm{C}]}$$

Note:

The steady-state approximation does not imply that $[\mathrm{X}]$ is even approximately constant, only that its absolute rate of change is very much smaller than that of $[\mathrm{A}]$ and $[\mathrm{D}]$. Since according to the reaction scheme $\frac{\mathrm{d}\,[\mathrm{D}]}{\mathrm{d}t} = k_2\,[\mathrm{X}]\,[\mathrm{C}]$, the assumption that $[\mathrm{X}]$ is constant would lead, for the case in which **C** is in large excess, to the absurd conclusion that formation of the product **D** will continue at a constant rate even after the reactant **A** has been consumed.

2. In a stirred flow reactor a steady state implies a regime so that all concentrations are independent of time.

Source:

PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1166

PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2298

See also:

PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 187

PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2216

Stefan–Boltzmann constant

Fundamental physical constant $\sigma = \frac{2\,\pi^5\,k^4}{15\,h^3\,c_0^{\,2}} = 5.670\,51(19) \times 10^{-8}\ \mathrm{W\ m^{-2}\ K^{-4}}$.

Source:

CODATA Bull. 1986, *63*, 1

stem cell

Multipotent cell with mitotic potential that may serve as a precursor for many kinds of differentiated cells.

Source:

PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1070

stem

in polymer crystals

A crystallized, rodlike portion of a polymer chain connected to non-rodlike portions, or chain ends, or both.

Source:
Purple Book, p. 83

step height

in chromatography

The distance perpendicular to the time or volume axis, through which the baseline moves as a result of a step on an integral chromatogram.

Source:
Orange Book, p. 96

step

in chromatography

The portion of an integral chromatogram recording the amount of a component, or the corresponding change in the signal from the detector as the component emerges from the column.

Source:
Orange Book, p. 96

stepwise elution

in chromatography

An elution process in which the composition of the mobile phase is changed in steps during a single chromatographic run.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 827
Orange Book, p. 92

stepwise reaction

A chemical reaction with at least one reaction intermediate and involving at least two consecutive elementary reactions.
See also: composite reaction

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1167
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 187

steradian

SI derived unit of solid angle, $\mathrm{sr} = 1$.

Source:
Green Book, 2nd ed., p. 72

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 993

stereoblock macromolecule

A block macromolecule composed of stereoregular, and possibly nonstereoregular, blocks.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2293

stereoblock polymer

A polymer composed of stereoblock macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2303

stereochemical formula (stereoformula)

A three-dimensional view of a molecule either as such or in a projection.
See: projection formula

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

stereochemical non-rigidity

The capability of a molecule to undergo fast and reversible intramolecular isomerization, the energy barrier to which is lower than that allowing for the preparative isolation of the individual isomers at room temperature. It is conventional to assign to the sterochemically non-rigid systems those compounds whose molecules rearrange rapidly enough to influence NMR line shapes at temperatures within the practical range (from $-100\ °\mathrm{C}$ to $200\ °\mathrm{C}$) of experimentation. The energy barriers to thus defined rearrangements fall into the range of $5\text{–}20\ \mathrm{kcal}/\mathrm{mol}$ ($21\text{–}85\ \mathrm{kJ}/\mathrm{mol}$).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1964

stereoconvergence

Also contains definition of: enantioconvergence

The predominant formation of the same stereoisomer or stereoisomer mixture of a reaction product when two different stereoisomers of the reactant are used in the same reaction. When that product involved in the reaction is one enantiomer the result has been called enantioconvergence.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

stereodescriptor

A prefix to specify configuration (absolute or relative) or conformation. For example *R*, *S*; *r*, *s*; *P*, *M*; *Re*, *Si*; *E*, *Z*; *ap*, *sp*; etc.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

stereoelectronic

Pertaining to the dependence of the properties (especially the energy) of a molecular entity in a particular electronic state (or of a transition state) on relative nuclear geometry. The electronic ground state is usually considered, but the term can apply to excited states as well. Stereoelectronic effects arise from the different alignment of electronic orbitals in different arrangements of nuclear geometry.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1167

stereoelectronic control

Control of the nature of the products of a chemical reaction (or of its rate) by stereoelectronic factors. The term is usually applied in the framework of an orbital approximation. The variations of molecular orbital energies with relative nuclear geometry (along a reaction coordinate) are then seen as consequences of variations in basis-orbital overlaps.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2218

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1167

stereogenic unit (stereogen/stereoelement)

A grouping within a molecular entity that may be considered a focus of stereoisomerism. At least one of these must be present in every enantiomer (though the presence of stereogenic units does not conversely require the corresponding chemical species to be chiral). Three basic types are recognized for molecular entities involving atoms having not more than four substituents:

1. A grouping of atoms consisting of a central atom and distinguishable ligands, such that the interchange of any two of the substituents leads to a stereoisomer. An asymmetric atom (chirality centre) is the traditional example of this stereogenic unit.
2. A chain of four non-coplanar atoms (or rigid groups) in a stable conformation, such that an imaginary or real (restricted) rotation (with a change of sign of the torsion angle) about the central bond leads to a stereoisomer.
3. A grouping of atoms consisting of a double bond with substituents which give rise to cis-trans isomerism.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2219

stereoheterotopic

Either enantiotopic or diastereotopic. (In contrast the term constitutionally heterotopic has been used to describe identical groups located in constitutionally non-equivalent positions).
See also: *pro-R*, *pro-S*

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2219

stereohomosequence

in a polymer

A configurational homosequence in which the relative or absolute configuration is defined at all sites of stereoisomerism in the main chain of a polymer molecule.

Source:
Purple Book, p. 36

stereoisomerism

Isomerism due to differences in the spatial arrangement of atoms without any differences in connectivity or bond multiplicity between the isomers.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2219

stereoisomers

Isomers that possess identical constitution, but which differ in the arrangement of their atoms in space.
See: enantiomer, diastereoisomer, cis-trans isomers

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2219

stereomutation

A change of configuration at a stereogenic unit brought about by physical or chemical means.
See: epimerization

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2219

stereoregular macromolecule

A regular macromolecule essentially comprising only one species of stereorepeating unit.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2292

stereoregular polymer

A polymer composed of stereoregular macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2302

stereorepeating unit

in a polymer

A configurational repeating unit having defined configuration at all sites of stereoisomerism in the main chain of a regular macromolecule, a regular oligomer molecule, a regular block or a regular chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2291

stereoselective polymerization

Polymerization in which a polymer molecule is formed from a mixture of stereoisomeric monomer molecules by incorporation of only one stereoisomeric species.

Source:
Purple Book, p. 19

stereoselective synthesis

A chemical reaction (or reaction sequence) in which one or more new elements of chirality are formed in a substrate molecule and which produces the stereoisomeric (enantiomeric or diastereoisomeric) products in unequal amounts. Traditionally called asymmetric synthesis.
See also: stereoselectivity

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2219

stereoselectivity

Also contains definition of: diastereoselectivity

The preferential formation in a chemical reaction of one stereoisomer over another. When the stereoisomers are enantiomers, the phenomenon is called enantioselectivity and is quantitatively expressed by the enantiomer excess; when they are diastereoisomers, it is called diastereoselectivity and is quantitatively expressed by the diastereoisomer excess.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2219

See also:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1167

stereosequence

in a polymer

A configurational sequence in which the relative or absolute configuration is defined at all sites of stereoisomerism in the main chain of a polymer molecule.

Source:
Purple Book, p. 36

stereospecific polymerization

Polymerization in which a tactic polymer is formed. However, polymerization in which stereoisomerism present in the monomer is merely retained in the polymer is not to be regarded as stereospecific. For example, the polymerization of a chiral monomer, e.g. D-propylene oxide (D-methyloxirane), with retention of configuration is not considered to be a stereospecific reaction; however, selective polymerization, with retention, of one of the enantiomers present in a mixture of D- and L-propylene oxide molecules is so classified.

Source:
Purple Book, p. 19
Purple Book, p. 32

stereospecifically labelled tracer

A tracer in which the label is present in a stereospecific position.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

stereospecificity (stereospecific)

1. A reaction is termed stereospecific if starting materials differing only in their configuration are converted into stereoisomeric products. According to this definition, a stereospecific process is necessarily stereoselective but not all stereoselective processes are stereospecific. Stereospecificity may be total (100%) or partial. The term is also applied to situations where reaction can be performed with only one stereoisomer. For example, the exclusive formation of *trans*-1,2-dibromocyclohexane upon bromination of cyclohexene is a stereospecific process, although the analogous reaction with (*E*)-cyclohexene has not been performed.
2. The term has also been applied to describe a reaction of very high stereoselectivity, but this usage is unnecessary and is discouraged.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1167
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2219

steric effect

The effect on a chemical or physical property (structure, rate or equilibrium constant) upon introduction of substituents having different steric requirements. The steric effect in a reaction is ascribed to the difference in steric energy between, on the one hand, reactants and, on the other hand, a transition state (or products). A steric effect on a rate process may result in a rate increase ('steric acceleration') or a decrease ('steric retardation'). (The adjective 'steric' is not to be confused with stereochemical.) Steric effects arise from contributions ascribed to strain as the sum of (1) non-bonded repulsions, (2) bond angle strain and (3) bond stretches or compressions. For the purpose of correlation analysis or linear free-energy relations various scales of steric parameters have been proposed, notably A values, Taft's E_{s} and Charton's ν scales. In a reactant molecule RY and an appropriate reference molecule $\mathrm{R^{o}Y}$, the 'primary steric effect' of R is the direct result of differences in compressions which

occur because R differs from R^o in the vicinity of the reaction centre Y . A 'secondary steric effect' involves the differential moderation of electron delocalization by non-bonded compressions. Some authors make a distinction between 'steric' effects attributed to van der Waals repulsions alone, and 'strain' effects, attributed to deviations of bond angles from 'ideal' values.
See: Taft equation, van der Waals forces

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1168

steric factor

A factor introduced into simple versions of the collision theory of reactions to take care of the fact that the reaction probability depends on the certain mutual orientations of the reactant molecules.
See also: collision frequency

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 187

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2216

steric factor

in polymers

The ratio, σ, of the root-mean-square end-to-end distance of a polymer chain with unperturbed dimensions, $< r^2 >_0^{1/2}$, to that of a freely rotating chain with the same structure, $< r^2 >_{0,f}^{1/2}$, i.e. $\sqrt{\frac{< r^2 >_0}{< r^2 >_{0,f}}}$, in the limit of infinite chain length. The steric factor reflects the effect of hindrance to free rotation.

Source:
Purple Book, p. 50

steric hindrance

The original term for a steric effect arising from crowding of substituents.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1168

steric isotope effect

A secondary isotope effect attributed to the different vibrational amplitudes of isotopologues. For example, both the mean and mean-square amplitudes of vibrations associated with C–H bonds are greater than those of C–D bonds. The greater effective bulk of molecules containing the former may be manifested by a steric effect on a rate or equilibrium constant.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1131

steric strain

1. ***See:*** strain

   Source:
   PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1077
2. ***See:*** angle strain
3. ***See:*** eclipsing strain
4. ***See:*** transannular strain

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2219

steric-approach control

Control of stereoselectivity of a reaction by steric hindrance towards attack of the reagent, which is directed to the less hindered face of the molecule. Partial bond making is strong enough at the transition state for steric control to take place. This suggests that the transition state should not be close to products.
See also: product development control

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1168

Stern layer

Counter and co-ions in immediate contact with a surface are said to be located in the Stern layer, and form with the fixed charge a molecular capacitor.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 618

Stern–Volmer kinetic relationships

This term applies broadly to variations of quantum yields of photophysical processes (e.g. fluorescence or phosphorescence) or photochemical reactions (usually reaction quantum yield) with the concentration of a given reagent which may be a substrate or a quencher. In the simplest case, a plot of $\frac{\Phi^0}{\Phi}$ (or $\frac{M^0}{M}$ for emission) vs. concentration of quencher, $[\mathrm{Q}]$, is linear obeying the equation:

$$\frac{\Phi^0}{\Phi} \text{ or } \frac{M^0}{M} = 1 + K_{\mathrm{sv}}\,[\mathrm{Q}]$$

In equation (1) K_{sv} is referred to as the Stern–Volmer constant. Equation (1) applies when a quencher inhibits either a photochemical reaction or a photophysical process by a single reaction. Φ^0 and M^0 are the quantum yield and emission intensity radiant exitance, respectively, in the absence of the quencher Q, while Φ and M are the same quantities in the presence of the different concentrations of Q. In the case of dynamic quenching the constant K_{sv} is the product of the true quenching constant k_{q} and the excited state lifetime, τ^0, in the absence of quencher. k_{q} is the bimolecular reaction rate constant for the elementary reaction of the excited state with the particular quencher Q. Equation (1) can therefore be replaced by the expression (2):

$$\frac{\Phi^0}{\Phi} \text{ or } \frac{M^0}{M} = 1 + k_{\mathrm{q}}\,\tau^0\,[\mathrm{Q}]$$

When an excited state undergoes a bimolecular reaction with rate constant k_{r} to form a product, a double-reciprocal relationship is observed according to the equation:

$$\frac{1}{\Phi_{\mathrm{p}}} = \left(1 + \frac{1}{k_{\mathrm{r}}\,\tau^0\ [\mathrm{S}]}\right)\frac{1}{A \cdot B}$$

where Φ_{p} is the quantum efficiency of product formation, A the efficiency of forming the reactive excited state, B the fraction of reactions of the excited state with substrate S which leads to product, and $[\mathrm{S}]$ is the concentration of reactive ground-state substrate. The intercept/slope ratio gives $k_{\mathrm{r}}\,\tau^0$. If $[\mathrm{S}] = [\mathrm{Q}]$, and if a photophysical process is monitored, plots of equations (2) and (3) should provide independent determinations of the product-forming rate constant k_{r}. When the lifetime of an excited state is observed as a function of the concentration of S or Q, a linear relationship should be observed according to the equation:

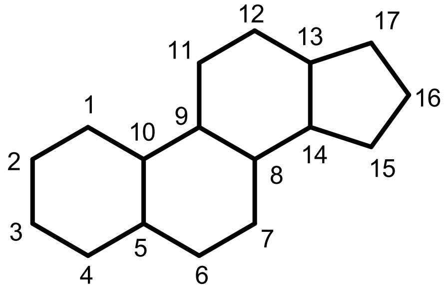
$$\frac{\tau^0}{\tau} = 1 + k_{\mathrm{q}}\,\tau^0\ [\mathrm{Q}]$$

where τ^0 is the lifetime of the excited state in the absence of the quencher Q.
See also: self-quenching

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2277

steroids

Naturally occurring compounds and synthetic analogues, based on the cyclopenta[*a*]phenanthrene carbon skeleton, partially or completely hydrogenated; there are usually methyl groups at C-10 and C-13, and often an alkyl group at C-17. By extension, one or more bond scissions, ring expansions and/or ring contractions of the skeleton may have occurred. Natural steroids are derived biogenetically from triterpenoids.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

See also:
White Book, p. 193

sterols

Natural products derived from the steroid skeleton and containing a hydroxy group in the 3 position, closely related to cholestan-3-ol.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

See also:
White Book, p. 193

stibanes

The saturated hydrides of tervalent antimony, having the general formula Sb_nH_{n+2}. Hydrocarbyl derivatives of SbH_3 belong to the class stibines.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

stibanylidenes

Also contains definition of: stibinidenes

Recommended name for carbene analogues having the structure RSb: (former IUPAC name is stibinediyls). A common non-IUPAC synonym is stibinidenes.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

stibines

SbH_3 and compounds derived from it by substituting one, two or three hydrogen atoms by hydrocarbyl groups R_3Sb. $RSbH_2$, R_2SbH and R_3Sb ($R \neq H$) are called primary, secondary and tertiary stibines, respectively. A specific stibine is preferably named as a substituted stibane. E.g. $(CH_2{=}CH)_3Sb$ trivinylstibane.
See: stibanes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

stibonium compounds

Salts (including hydroxides) containing an atom of tetracoordinate antimony, of the form $[R_4Sb]^+X^-$.
See: onium compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

sticking coefficient

in surface chemistry

The ratio of the rate of adsorption to the rate at which the adsorptive strikes the total surface, i.e. covered and uncovered. It is usually a function of surface coverage, of temperature and of the details of the surface structure of the adsorbent.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 78

sticking probability

in surface chemistry

Often used with the same meaning as sticking coefficient, but in principle it is a microscopic quantity concerned with the individual collision process.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 78

sticky ends

in biotechnology

The staggered ends of complementary sequences of DNA which result from cleavage by restriction enzymes.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 166

stimulated emission

That part of the emission which is induced by a resonant perturbing electromagnetic field. The transition between states, n and m, is governed by the Einstein coefficient of stimulated emission, B_{nm}. CIDNP emission and lasing action are examples of processes which require stimulated emission.
See also: spontaneous emission

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2279

stirred flow reactor

in catalysis

A reactor within which effective mixing is achieved, often by placing the catalyst in a rapidly-rotating basket.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 80

stochastic effect

Consequence for which the probability of occurrence depends on the absorbed dose; hereditary effects and cancer induced by radiation are considered to be stochastic effects. The term 'stochastic' indicates that the occurrence of effects so named would be random. This means that, even for an individual, there is no threshold of dose below which there is absolutely no probability of an effect occurring, and the chance of experiencing the effect increases with increasing dose.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1023

stochastic sampling

Synonymous with random sampling.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2216

stochastic theories

Theories that treat reaction rates in terms of the probabilities of transitions between the various energy levels in the reactant molecules.

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 767

Stock number [obsolete]

Usage not recommended.
See: oxidation number

Source:
Red Book, p. 66
Red Book, p. 148

Stockholm convention

IUPAC convention on signs of electromotive forces and electrode potentials.

Source:
Physical Chemistry Division, unpublished.

stoichiometric

Involving chemical combination in simple integral ratios. Characterized by having no excess of reactants or products over that required to satisfy the balanced chemical equation representing the given chemical reaction.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2216

stoichiometric concentration, c

The stoichiometric concentration, c_{B}, of a component B in a system is given by the expression:

$$c_{\mathrm{B}} = \frac{n_{\mathrm{B}}}{V}$$

where n_{B} is the stoichiometric amount of substance of component B in the system and V is the volume of the system. The component added to the system may dissociate or react with other components to form a series of derived components and only a fraction of the original component may actually exist in a free form in the system. It is therefore essential to distinguish between the stoichiometric concentration and the amount-of-substance concentration of the free form of the component in the system. Sometimes stoichiometric quantities are indicated by a subscript ($_{\mathrm{o}}$), e.g. $n_{\mathrm{o,B}}$, $c_{\mathrm{o,B}}$. In clinical chemistry, the term stoichiometric concentration is rarely employed. Instead, the name of the component is modified to indicate inclusion of the various derived forms, e.g. mixtures of a defined chemical component and its derivatives may be denoted by the plural form of the name of the pure unchanged substance, or to indicate the sum of components specified in individual quantities the specification 'total' may be employed.

Source:
PAC, 1984, *56*, 567 *(Physicochemical quantities and units in clinical chemistry with special emphasis on activities and activity coefficients (Recommendations 1983))* on page 568

stoichiometric mean molal (practical activity coefficient)

in electrochemistry

The practical activity coefficient of electrolyte B is given by

$$\gamma_{\pm} = \frac{a_{\pm}}{\sqrt{\nu_{+}^{\nu_{+}}\,\nu_{-}^{\nu_{-}}}\,\frac{m_{\mathrm{B}}}{m^{+}}}$$

where $a_{\pm}$ is the mean activity of B in solution, m_{B} is the molality of B, $m^{+} = 1\ \mathrm{mol\ kg^{-1}}$, ν_{+} is the number of cations and ν_{-} the number of anions in the chosen group B which is taken as the electrolyte.

$$\nu = \nu_{+} + \nu_{-}$$

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 510

stoichiometric number, ν

A chemical reaction of known stoichiometry can be written in general as:

$$a\mathrm{A} + b\mathrm{B} + \ldots \rightarrow \ldots + y\mathrm{Y} + z\mathrm{Z}$$

For the reaction products Y and Z the numbers y and z are known as the stoichiometric numbers, ν_{Y} and ν_{Z}, for Y and Z respectively. For the reactants the stoichiometric numbers are the negatives of the numbers appearing in the equation; for example the stoichiometric number ν_{A} for the reactant A is $-a$. In other words, the stoichiometric numbers are positive for products and negative for reactants.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 187
Green Book, 2nd ed., p. 42
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 993

See also:
PAC, 1996, *68*, 1167 *(Pesticides report 36. Glossary of terms relating to pesticides (IUPAC Recommendations 1996))* on page 1168

stoichiometry

The term refers to the relationship between the amounts of substances that react together in a particular chemical reaction, and the amounts of products that are formed. The general stoichiometric equation:

$$a\mathrm{A} + b\mathrm{B} + \ldots \rightarrow \ldots + y\mathrm{Y} + z\mathrm{Z}$$

provides the information that *a* moles of A reacts with *b* moles of B to produce *y* moles of Y and *z* moles of Z. The stoichiometry of a reaction may be unknown, or may be very complex. For example, the thermal decomposition of acetaldehyde yields mainly methane and carbon monoxide, but also a variety of minor products such as ethane, acetone and diacetyl. The stoichiometric equation:

$$\mathrm{CH_3CHO} \longrightarrow \mathrm{CH_4} + \mathrm{CO}$$

is therefore only an approximate one. Even when the overall stoichiometry of a reaction is well defined, it may be time-dependent in that it varies during the course of a reaction. Thus if a reaction occurs by the mechanism $\mathrm{A} \rightarrow \mathrm{X} \rightarrow \mathrm{Y}$, and X is formed in substantial amounts during the course of the process, the relationship between the amounts of A, X and Y will vary with time, and no one stoichiometric equation can represent the reaction at all times.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 187

stokes

cgs unit of kinematic viscosity, $\mathrm{St} = 10^{-4}\ \mathrm{m}^2\ \mathrm{s}^{-1}$.

Source:
Green Book, 2nd ed., p. 112
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 993

Stokes law

$F = 6\,\pi\,\eta\,r\,v$, where F is the force exerted on a sphere of radius r which is moving through a fluid of viscosity η with a relative velocity v; this equation holds at low velocities which are free from turbulence (called the Stokes region).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2216

Stokes number, *St*

Sometimes referred to as the inertial parameter; it is an index of the impactability of an aerosol particle. It is defined by the equation: $St = 2\,\tau\,(V_{\mathrm{t}} - v_{\mathrm{t}})\,D_{\mathrm{p}}$ where D_{p} is the diameter of a small drop, $V_{\mathrm{t}} - v_{\mathrm{t}}$ is the difference in fall velocities of the drop and aerosol particles and τ is the characteristic relaxation time of a particle.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2216

Stokes parameters

Of elliptically polarized incident radiation, these are given by

$$s_0^0 = E_1^0 + E_2^0$$

$$s_1^0 = E_1^0 - E_2^0$$

$$s_2^0 = 2\sqrt{E_1^0 E_2^0}\,\cos\delta^0$$

$$s_3^0 = 2\sqrt{E_1^0 E_2^0}\,\sin\delta^0$$

where E_1^0 and E_2^0 specify the irradiances of the incident light polarized with their electric vectors vibrating perpendicular and parallel to the scattering, respectively and δ^0 is the phase difference between these electric vectors.
See also: scattering matrix

Source:
PAC, 1983, *55*, 931 *(Definitions, terminology and symbols in colloid and surface chemistry. Part 1.14: Light scattering (Provisional))* on page 933

Stokes shift

Also contains definition of: anti-Stokes shift

The difference (usually in frequency units) between the spectral positions of the band maxima (or the band origin) of the absorption and luminescence arising from the same electronic transition. Generally, the luminescence occurring at a longer wavelength than the absorption is stronger than the opposite. The latter may be called an anti-Stokes shift.
See: coherent radiation

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2278

Stokes type radiation

Fluorescence radiation occurring at wavelengths longer than absorption, i.e. the normal case, is said to be of the Stokes type.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 236

stopped flow

A technique for following the kinetics of reactions in solution (usually in the millisecond time range) in which two reactant solutions are rapidly mixed by being forced through a mixing chamber. The flow of the mixed solution along a uniform tube is then suddenly arrested. At a fixed position along the tube the solution is monitored (as a function of time following the stoppage of the flow) by some method with a rapid response (e.g. photometry).
See: mixing control

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1168
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2298

stopped-flow cell

in spectrochemical analysis

A small-volume absorption cell connected to a rapid mixing chamber.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1454

stopping power

Of a substance, for charged particles of specified energy, the average energy loss in passing through a thin layer of that substance, divided by the thickness of that layer.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1553

STP

Abbreviation for standard temperature ($273.15\ \mathrm{K}$ or $0\ °\mathrm{C}$) and pressure ($10^5\ \mathrm{Pa}$); usually employed in reporting gas volumes. Note that flow meters calibrated in standard gas volumes per unit time often refer to volumes at $25\ °\mathrm{C}$, not $0\ °\mathrm{C}$.
See also: standard conditions for gases

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2217

strain

Strain is present in a molecular entity or transition structure if the energy is enhanced because of unfavourable bond lengths, bond angles or dihedral angles ('torsional strain') relative to a standard. It is quantitatively defined as the standard enthalpy of a structure relative to a strainless structure (real or hypothetical) made up from the same atoms with the same types of bonding. (The enthalpy of formation of cyclopropane is $53.6\ \mathrm{kJ\ mol^{-1}}$, whereas the enthalpy of formation based on three 'normal' methylene groups, from acyclic models, is $-62\ \mathrm{kJ\ mol^{-1}}$. On this basis cyclopropane is destabilized by *ca.* $115\ \mathrm{kJ\ mol^{-1}}$ of strain energy.)
See: molecular mechanics calculation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1168

strain energy

The excess energy due to steric strain of a molecular entity or transition state structure, *i.e.* distortions relative to a reference (real or hypothetical) 'strainless' structure with the standard bond lengths, bond angles and dihedral angles. The strain energy components involve the following destabilizing terms: non-bonded repulsions, bond-angle distortions, bond stretch or compression, rotation around or twisting of double bonds, and electrostatic strain. In general, the contributions of these components are inseparable and interdependent. A quantitative assessment of strain and strain energies can be made by taking the difference between the heat of formation of the substance under consideration and that of a hypothetical strain-free model. Several approaches to the assessment of strain energies have been developed based on the use of energies of isodesmic and homodesmotic reactions and on the so-called 'strainless increments', *i.e.* heats of formation of certain groups (CH_3, CH_2, CH, C *etc*).

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1964

strain-induced transition

A transition in a solid that is initiated by plastic strain.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 591

stratified film

A film in which more than two thicknesses coexist in a fixed configuration over significant periods of time.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 614

stratified sample

A sample consisting of portions obtained from identified subparts (strata) of the parent population. Within each stratum, the samples are taken randomly. The objective of taking stratified samples is to obtain a more representative sample than that which might otherwise be obtained by random sampling.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1203

stratocumulus cloud

A layer of patches composed of laminae or globular masses arranged in groups, lines or waves and having a soft, grey appearance; very often the rolls are so close together that their edges join and give the undersurface a wavy character; the process of formation (cumulogenesis) involves the spreading out of the tops of cumulus clouds, the latter having disappeared; $< 2000\ \mathrm{m}$; usually warmer than $-5\ ^\circ\mathrm{C}$; vertical velocities usually $< 0.1\ \mathrm{m\ s^{-1}}$.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

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NOTE:
An error in this entry in the printed version of the Compendium (omission of a minus sign) has been corrected.

stratopause

That region of the atmosphere which lies between the stratosphere and the mesosphere and in which a maximum in the temperature occurs.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2216

stratosphere

The atmospheric shell lying just above the troposphere which is characterized by an increasing temperature with altitude. The stratosphere begins at the tropopause (about $10 - 15\ \mathrm{km}$ height) and extends to a height of about $50\ \mathrm{km}$, where the lapse rate changes sign at the stratopause and the beginning of the mesosphere.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2217

stratus cloud

A uniform, featureless layer of cloud resembling fog but not resting on the ground; when this very low layer is broken up into irregular shreds, it is designated as fractostratus; $300\ \mathrm{m} - 600\ \mathrm{m}$; widespread irregular stirring and lifting of the shallow layer of cool, damp air near the ground.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2180

stray radiation error

in spectrochemical analysis

A spectrometer set to pass radiation of a particular wavelength band always has a small amount of stray radiation of other wavelengths. Since the sample may absorb more (or less) of this stray radiation than of the radiation at the selected wavelength an error can occur. This error is called a stray radiation error.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1456

streak tube

Also contains definition of: streak camera

An image converter adapted to provide scanning or time-resolved images. If the image is recorded the whole device is an example of a streak camera.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1758

streaming birefringence

Synonym: flow birefringence

The birefringence induced by flow in liquids, solutions and dispersions of optically anisotropic, anisometric or deformable flow molecules or particles due to a non-random orientation of the molecules or particles. Synonymous with flow birefringence.

Source:
Purple Book, p. 61

streaming current

The electric current I flowing in a streaming cell if the electrodes, which are supposed to be ideally depolarized, are short-circuited. I is positive if the current in the membrane, plug, etc., is from high to low pressure side (and in the outside lead from low to high pressure side).

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

streaming potential difference (streaming potential)

The potential difference E_{st} or E at zero current caused by the flow of liquid under a pressure gradient through a membrane, plug or capillary. Identical electrodes must be used on both sides of the membrane, plug, etc. E is positive if the higher potential is on the high pressure side.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 620

stress graphitization

The solid-state transformation of non-graphitic carbon into graphite by heat treatment combined with application of mechanical stress, resulting in a defined degree of graphitization being obtained at a lower temperature and/or after a shorter time of heat treatment than in the absence of applied stress.
Note:

Stress graphitization may also occur in volume elements of a carbon body in the process of heat treatment as a result of the action of internal residual or thermal stresses.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 505

stress-assisted transition

A transition that takes place when an applied stress assists the transition to the new phase.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 591

stripping

The process of removing solute(s) from a loaded solvent or extract. Generally this refers to the main solute(s) present.
Notes:
1. Where appropriate, e.g. when liquid-liquid distribution is used for stripping, the term back-extraction can be used. The terms back-washing and re-extraction are not recommended.
2. The recent application of selective stripping of solutes as a separation method leads to some confusion between the terms stripping and scrubbing. It is recommended that the term scrubbing be reserved for the operation of removing contaminants (impurities) from an extract (where the scrub raffinate is often recycled to the loading step) and the term selective stripping be used where two or more main solutes are stripped successively from an extract, usually with different stripping agents, with a view to their subsequent separate recovery from solution for analysis.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2390
Orange Book, p. 91

stripping isotherm

See: distribution isotherm
Note:
In the graphical representation of stripping isotherms, the axes are often interchanged from those used to represent the phases for extraction isotherms. It is essential that the axes be clearly labelled.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2391

stripping ratio

in solvent extraction

See: distribution ratio

Notes:

1. This term is usually defined as the inverse ratio to the distribution ratio, i.e. in aqueous-organic systems the aqueous phase concentration of solute is the numerator and the organic phase concentration is the denominator. Their usage should be clearly defined.
2. The term stripping coefficient is not recommended.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2391

stripping reaction

A chemical process, studied in a molecular beam, in which the reaction products are scattered forward with respect to the moving centre of mass of the system.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 188

stripping solution

in liquid-liquid distribution

A solution (usually aqueous, sometimes water alone) used for back-extracting the distribuend from the extract (usually organic).

Source:
Orange Book, p. 91

strong collision

A collision between two molecules in which the amount of energy transferred from one to the other is large compared with $k_B T$, where k_B is the Boltzmann constant and T the absolute temperature.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 188

structural disorder

Any deviation from the ideal three-dimensional regularity of the crystal structure.

Source:
Purple Book, p. 79

structural formula

A formula which gives information about the way the atoms in a molecule are connected and arranged in space.

Source:
Red Book, p. 46

structural stability

Within the Born–Oppenheimer (adiabatic) approximation, this is associated with an energy minimum on a potential energy surface. Structural stability implies that any change in the coordinates of the nuclei can only increase the total energy.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1964

structural transition

A reversible or irreversible transition that involves a change of the crystal structure. Example: The transition of NH_4Cl at 469 K from a CsCl-type structure to a NaCl-type structure.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 591

structure

of a catalyst

The distribution in space of the atoms or ions in the material part of the catalyst and, in particular, the distribution at the surface.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

structure-based design

in drug design

Structure-based design is a design strategy for new chemical entities based on the three-dimensional (*3D*) structure of the target obtained by X-ray or nuclear magnetic resonance (*NMR*) studies, or from protein homology models.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1150

structure-property correlations (SPC)

Structure-property correlations (*SPC*) refer to all statistical mathematical methods used to correlate any molecular property (intrinsic, chemical or biological) to any other property, using statistical regression or pattern recognition techniques.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1150

structure–activity relationship (SAR)

Association between specific aspects of molecular structure and defined biological action.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1071

styphnates

Salts or charge-transfer complexes of styphnic acid (2,4,6-trinitrobenzene-1,3-diol).
See: picrates

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

subchain

of a polymer

An arbitrarily chosen contiguous sequence of constitutional units in a chain.
Note:
The term 'subchain' may be used to define designated subsets of the constitutional units in a chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2293

subgroup-supergroup transition

A transition in which the space-group symmetry of the lower symmetry phase is a subgroup of that of the higher symmetry phase. Example: The transition of the low-temperature polymorph of quartz characterized by space-group symmetry $P3_12$ (trigonal), to the high temperature polymorph of quartz with space-group symmetry, $P6_222$ (hexagonal). Synonymous with symmetry-breaking transition (note: this term, strictly speaking, is no longer in use).

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 591

subjacent orbital

Also contains definition of: NHOMO

The *N*ext-to-*H*ighest *O*ccupied *M*olecular *O*rbital ('NHOMO', also called 'HOMO') and the *S*econd *L*owest *U*noccupied *M*olecular *O*rbital (SLUMO). Subjacent orbitals are sometimes found to play an important role in the interpretation of molecular interactions according to the frontier orbital approach.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169

sublation

in solvent extraction

A flotation process in which the material of interest, adsorbed on the surface of gas bubbles in a liquid, is collected on an upper layer of immiscible liquid. There is no liquid-phase mixing in the bulk of the system; as a result recoveries can approach 100%.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2379

sublimation

The direct transition of a solid to a vapour without passing through a liquid phase. Example: The transition of solid CO_2 to CO_2 vapour.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 591

subsample

A subsample may be: (a) a portion of the sample obtained by selection or division; (b) an individual unit of the lot taken as part of the sample; (c) the final unit of multistage sampling. The term 'subsample' is used either in the sense of a 'sample of a sample' or as a synonym for 'unit'. In practice, the meaning is usually apparent from the context or is defined.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1205

substance concentration

See: amount *of substance* concentration

Source:
Green Book, 2nd ed., p. 42

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 994

substance content, n / m

Amount-of-substance of a component divided by the mass of the system.
Notes:
1. The term component is recommended for clinical chemistry, ISO uses "substance".
2. The term system is recommended for clinical chemistry, ISO uses mixture.
3. Use of the term level as a synonym for content is deprecated.
4. In describing a quantity, content must be clearly differentiated from concentration.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 994

substance flow rate

Amount-of-substance of a component crossing a surface divided by the time. For clinical chemistry the term component is recommended. ISO uses "substance".

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 994

substance fraction, x

Ratio of the amount-of-substance of the component to the total amount-of-substance in the system containing the component.
Notes:
1. The term substance fraction is recommended for clinical chemistry, IUPAC also uses mole fraction and amount fraction.
2. For clinical chemistry the term component is recommended, ISO uses "substance".
3. For clinical chemistry the term system is recommended, ISO uses mixture.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 994

substituent atom (group)

An atom (group) that replaces one or more hydrogen atoms attached to a parent structure or characteristic group except for hydrogen atoms attached to a chalcogen atom.

Source:
Blue Book (Guide), p. 13
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169

substituent electronegativity

See: electronegativity

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169

substitution reaction

A reaction, elementary or stepwise, in which one atom or group in a molecular entity is replaced by another atom or group. For example,

$$CH_3{-}Cl + OH^- \longrightarrow CH_3{-}OH + Cl^-$$

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169

substitutive name

A name which indicates the exchange of one or more hydrogen atoms attached to a skeletal atom of a parent structure or to an atom of a characteristic group for another atom or group, which may be expressed by a suffix or by prefixes.

Source:
Blue Book (Guide), p. 15

substoichiometric extraction

Solvent extraction in which the amount of reagent used is lower than that dictated by stoichiometry. If the constants of formation and extraction of the complexes are high, the amount of extracted metal is dictated by the amount of extractant introduced.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2379

substoichiometric isotope dilution analysis

A kind of isotope dilution analysis in which the final isotopic abundance is estimated from the amount of the nuclide present in a known quantity of the relevant element separated from the test portion, where this quantity is smaller than the total amount of that element present in the test portion.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

substrate

A chemical species, the reaction of which with some other chemical reagent is under observation (e.g. a compound that is transformed under the influence of a catalyst). The term should be used with care. Either the context or a specific statement should always make it clear which chemical species in a reaction is regarded as the substrate.
See also: transformation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169
PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2298

substrate

in biocatalysis

1. The chemical entity whose conversion to a product or products is catalysed by one or several enzymes.
2. A solution or dry mixture containing all ingredients which are necessary for the growth of a microbial culture or for product formation.
3. Component in the nutrient medium, supplying the organisms with carbon (C-substrate), nitrogen (N-substrate), etc.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 166

substrate

Also contains definition of: subphase *in thin films*

in thin films

The terms substrate and subphase refer to a condensed phase that physically supports a film or layer. The term substrate should be used with care in the light of the existing double meaning of the term substrate in film science and technology, on the one hand, and in biochemistry, on the other. The term subphase applies, mainly, to a liquid phase underlying an adsorption layer or a floating spread monolayer.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1671

subtractive name

A name for a modified parent structure in which prefixes and/or suffixes indicate the removal of atoms or groups and, where required, replacement by an appropriate number of hydrogen atoms.

Source:
Blue Book (Guide), p. 16

successor complex

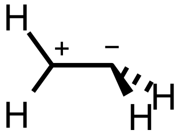
The radical ion pair which forms by the transfer of an electron from the donor D to the acceptor A after these species have diffused together to form the precursor or encounter complex:

$$A + D \rightarrow (A\,D) \rightarrow (A^{\bullet -}D^{\bullet +})$$

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169

sudden polarization

The occurrence of a large intramolecular charge separation in the singlet excited state of polyenes and their derivatives twisted about a double bond. Non-symmetrical substitution or geometrical distortion is effective in polarizing the system. An example is the stabilization of the zwitterionic structure of 90° twisted ethene with one methylene group pyramidalized:



Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1964

sugars

A loose term applied to monosaccharides and lower oligosaccharides.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

sulfamic acids

$H_2NS(=O)_2OH$ (sulfamic acid) and its N-hydrocarbyl derivatives. Sulfamic acid is called sulfamidic acid in inorganic chemistry.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

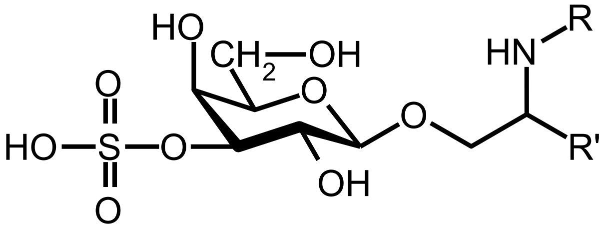
sulfanes [obsolete]

A term including hydropolysulfides, polysulfanes, polysulfides. Use is discouraged because of confusion with the newer systematic name sulfane, H_2S, and the numerous names derived therefrom.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

sulfatides

Hydrogen sulfate esters of glycosphingolipids. Specific compounds should be named as glycerosphingolipid derivatives, e.g.



R = fatty acid acyl group or H

R' = $CH_3[CH_2]_{14}CH(OH)$-

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1367

See also:
White Book, p. 187

sulfenamides

Compounds derived from sulfenic acids, RSOH (R ≠ H), by replacement of –OH by $-NR_2$. May alternatively be considered as alkylsulfanylamines, e.g. $C_2H_5SNH_2$ ethanesulfenamide or ethylsulfanylamine.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfenes

S,S-Dioxides of thioaldehydes and thioketones, $R_2C{=}SO_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfenic acids

Compounds having the structure RSOH ($R \neq H$), e.g. PhSOH benzenesulfenic acid.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfenium ions

A term sometimes erroneously used for sulfenylium ions.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfenyl groups

Groups having the structure RS– ($R \neq H$). This term is derived from sulfenic acids. The synonymous term sulfanyl groups is derived from sulfane, H_2S. E.g. CH_3–S– methanesulfenyl, methylthio or methylsulfanyl.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfenyl radicals

Sulfur-centered radicals having the structure $RS^{\cdot}$ ($R \neq H$). This term is derived from sulfenic acids. The synonymous term sulfanyl radicals is derived from sulfane, H_2S. E.g. $CH_3S^{\cdot}$ methylsulfanyl or methanesulfenyl radical. An older synonymous term is alkylthio radical.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfenylium ions

Cations having the structure RS^+ ($R \neq H$). This term is derived from sulfenic acids. The synonymous term sulfanylium ions is derived from sulfane, H_2S. E.g. CH_3S^+ methylsulfanylium or methanesulfenylium ion.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfides

1. Compounds having the structure RSR ($R \neq H$). Such compounds were once called thioethers.
   See also: thioacetals
2. In an inorganic sense, salts or other derivatives of hydrogen sulfide.
3. A term used in additive nomenclature, see imides (2).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfilimines

See: sulfimides (1)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfimides

1. $H_2S{=}NH$, sulfimide, and its hydrocarbyl derivatives. They are thus related to sulfoxides in the same way that imines are related to aldehydes or ketones, e.g. $(C_2H_5)_2S{=}NPh$ *S,S*-diethyl-*N*-phenylsulfimide.
2. A term used in Chemical Abstracts Service Index Nomenclature for sulfonylamines, $RN{=}S({=}O)_2$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfimines **[obsolete]**

A non-recommended synonym for sulfimides (1).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfinamides

Amides of sulfinic acids, RS(=O)OH; thus $RS(=O)NR_2$, e.g. $PhS(=O)NHCH_3$ *N*-methylbenzenesulfinamide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfinamidines

Amidines of sulfinic acids, RS(=O)OH; thus $RS(=NR)NR_2$, e.g. $PhS(=NH)NH_2$ benzenesulfinamidine.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1368

sulfines **[obsolete]**

S-Oxides of thioaldehydes and thioketones. Not recommended because in English the -ine termination should be reserved for amines, imines, etc., e.g. PhC(=S=O)H thiobenzaldehyde *S*-oxide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfinic acids

HS(=O)OH, sulfinic acid, and its *S*-hydrocarbyl derivatives, e.g. $(CH_3)_2CHS(=O)OH$ propane-2-sulfinic acid.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfinic anhydrides

Compounds having the structure RS(=O)OS(=O)R.
See also: acid anhydrides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfinimines **[obsolete]**

An obsolescent term for sulfimides (1).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfinylamines

Synonym: thionylamines

Compounds having the structure RN=S=O. Formerly called thionylamines.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfolipids

Sulfate esters of glycolipids.
See also: sulfatides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfonamides

Amides of sulfonic acids $RS(=O)_2NR'_2$, e.g. $PhS(=O)_2NHCH_3$ *N*-methylbenzenesulfonamide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfonamidines [obsolete]

A term abandoned because of its ambiguous use to mean either $RS(=O)=NH_2$ (sulfonimidamide) or $RS(=NH)_2=NH_2$ (sulfonodiimidamide).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfonediimines

Compounds having the structure, $RS(=NR)_2R$, formally derived from sulfones by replacing $(=O)_2$ by $(=NR)_2$, e.g. $Ph_2S(=NH)_2$ diphenyl sulfonediimine.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfones

Compounds having the structure, $RS(=O)_2R$ ($R \neq H$), e.g. $C_2H_5S(=O)_2CH_3$ ethyl methyl sulfone.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfonic acids

$HS(=O)_2OH$, sulfonic acid, and its *S*-hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfonic anhydrides

Compounds having the structure $RS(=O)_2OS(=O)_2R'$, e.g. $PhS(=O)_2OS(=O)_2Ph$ benzenesulfonic anhydride.
See also: acid anhydrides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

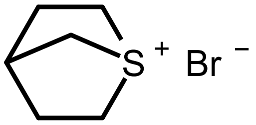
sulfonimides **[obsolete]**

A seldom used synonym of sulfoximides; its use is discouraged.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfonium compounds

Compounds having the structure R_3S^+ and associated anion (generally, but not necessarily, all three R groups are hydrocarbyl). E.g. $[(CH_3)_3S]^+Cl^-$, trimethylsulfonium chloride, or

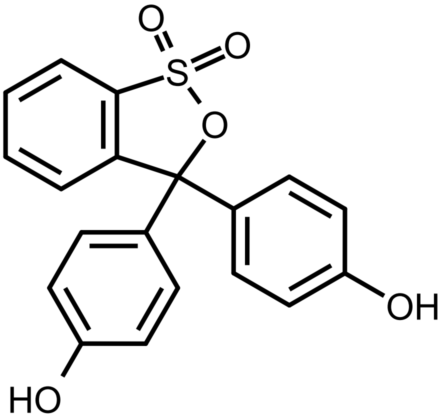


See: onium compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1369

sulfonphthaleins

3,3-Bis(hydroxyaryl)-3*H*-2,1-benzoxathiole *S,S*-dioxides, formed by condensation of *o*-sulfobenzoic acid with phenols or related compounds, e.g.



See: phthaleins

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

sulfonylamines

Compounds having the structure RN=S(=O)$_2$. (Indexed by Chemical Abstracts Service at the heading sulfimide). E.g. CH$_3$N=S(=O)$_2$ *N*-sulfonylmethylamine.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

sulfoxides

Compounds having the structure R$_2$S=O (R $\neq$ H), e.g. Ph$_2$S=O diphenyl sulfoxide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

sulfoximides

Synonym: sulfoximines

Compounds having the structure R$_2$S(=O)=NR. (Indexed by Chemical Abstracts Service at the heading sulfoximines). E.g. (CH$_3$)$_2$S(=O)=NPh *S,S*-dimethyl-*N*-phenylsulfoximide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

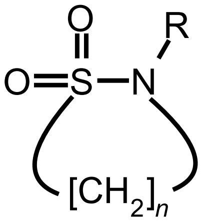
sulfur diimides

The parent compound HN=S=NH and hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

sultams

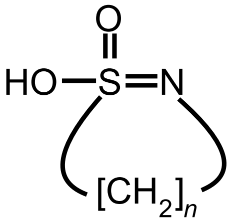
Sulfonamides in which the S-N bond is part of a ring.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

sultims

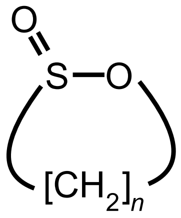
Tautomeric forms of sultams, having a sulfur–nitrogen double bond as part of a ring.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

sultines

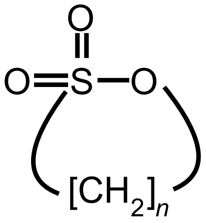
Intramolecular cyclic esters of hydroxy sulfinic acids. (Named by supposed analogy with lactones and sultones; but the -ine ending is unfortunate).



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

sultones

Intramolecular cyclic esters of hydroxy sulfonic acids, analogous to lactones.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

sum of states, $P(\varepsilon)$

The total number of states for a system corresponding to an energy ε less than or equal to a specified value.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 188

summit current

in polarography

In ac polarography, differential pulse polarography, derivative polarography, square-wave polarography, and similar techniques, the maximum value of the component of the current that is associated with the presence of a substance B. Normally this component of the current is faradaic, and the maximum arises because the rate of variation (with applied potential) of the rate of the charge-transfer process passes through a maximum. Similar maxima arise when this component is non-faradaic (and when B is surface-active rather than electroactive). In a case known to be of the latter type, the term apex current is recommended as being more specific.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1499

summit potential

In ac polarography, differential pulse polarography, derivative polarography, and similar techniques, the potential of the indicator electrode at which the summit current is attained.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1503

superabsorbent polymer

Polymer that can absorb and retain extremely large amounts of a liquid relative to its own mass.
Notes:

1. The liquid absorbed can be water or an organic liquid.
2. The swelling ratio of a superabsorbent polymer can reach the order of 1000:1.
3. Superabsorbent polymers for water are frequently polyelectrolytes.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 903

superacid

Also contains definitions of: magic acid, superbase

A medium having a high acidity, generally greater than that of 100 wt.% sulfuric acid. The common superacids are made by dissolving a powerful Lewis acid (e.g. SbF_5) in a suitable Brønsted acid such as HF or HSO_3F. (An equimolar mixture of HSO_3F and SbF_5 is known by the trade name 'magic acid'.) In a biochemical context 'superacid catalysis' is sometimes used to denote catalysis by metal ions analogous to catalysis by hydrogen ions. By analogy, a compound having a very high basicity, such as lithium diisopropylamide, is called a 'superbase'.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169

superconducting transition

A transition at the critical temperature, T_c, below which the resistance of electrical conductors becomes zero and magnetic flux is excluded. Examples: The transitions of Nb_3Sn, Nb_3Al and V_3Si to superconductors ($15\ K < T_c < 20\ K$) and $YBa_2Cu_3O_{7-x}$ ($x \approx 0.2$) at 90 K.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 592

supercritical drying of a gel

Drying of a gel using a supercritical fluid.
Note:
Since liquid and vapour are indistinguishable in a supercritical fluid, there is no capillary pressure to cause shrinkage and cracking of the pores formed in the gel.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1826

supercritical fluid

The defined state of a compound, mixture or element above its critical pressure (p_c) and critical temperature (T_c).

Source:
PAC, 1993, *65*, 2397 *(Nomenclature for supercritical fluid chromatography and extraction (IUPAC Recommendations 1993))* on page 2399

supercritical fluid chromatography (SFC)

A separation technique in which the mobile phase is a fluid above and relatively close to its critical temperature and pressure. In general the terms and definitions used in gas or liquid chromatography are equally applicable to supercritical fluid chromatography.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 825

superequivalent adsorption

This occurs when the specifically adsorbed amount of charge in the inner Helmholtz plane is higher than the charge on the metal phase, taken with the reverse sign.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 448

superexchange interaction

Electronic interaction between two molecular entities mediated by one or more different molecules or ions.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2279

superficial work

in surface chemistry

The reversible work of formation of unit area of new surface by cleavage. It has previously been called specific surface work, surface energy, surface tension or surface free energy. The symbol recommended is γ_{π} in preference to σ because of the confusion with surface charge density. The superficial work γ_{π} is a scalar quantity and consequently is isotropic.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1265

superlattice

Also contains definition of: quantum well multilayer

A periodic multilayer which is synthetic and where a unit cell, consisting of successive layers that are chemically different from their adjacent neighbours, is repeated. The term quantum well multilayer applies to the superlattices with artificially created electronic band structures.

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1672

superposability

The ability to bring two particular stereochemical formulae (or models) into coincidence (or to be exactly superposable in space, and for the corresponding molecular entities or objects to become exact replicas of each other) by no more than translation and rigid rotation.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2220

superradiance

Spontaneous emission amplified by a single pass through a population inverted medium. It is distinguished from true laser action by its lack of coherence. The term superradiance is frequently used in laser technology.
See: coherent radiation

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2279

supersaturation

1. In chemistry, an unstable system which has a greater concentration of a material in solution than would exist at equilibrium is said to be supersaturated.
2. In meteorology, supersaturation of an air mass with respect to H_2O vapour is of special interest. It is the saturation ratio minus one, or the percent supersaturation is the percent relative humidity minus 100.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2217

See also:
Orange Book, p. 84

support

of a catalyst

In multiphase catalysts, the active catalytic material is often present as the minor component dispersed upon a support sometimes called a carrier. The support may be catalytically inert but it may contribute to the overall catalytic activity.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

support plate

in chromatography

The plate that supports the thin layer in thin-layer chromatography.

Source:
Orange Book, p. 98

support-coated open-tubular (SCOT) column

in chromatography

A version of a porous-layer open-tabular (PLOT) column in which the porous layer consists of support particles and was deposited from a suspension.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831

supporting electrolyte

An electrolyte solution, whose constituents are not electroactive in the range of applied potentials being studied, and whose ionic strength (and, therefore, contribution to the conductivity) is usually much larger than the concentration of an electroactive substance to be dissolved in it.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1501

suppressor

A substance which reduces emission, absorption, or light scattering by an interferent, thus removing or lowering spectral interference.

Source:
Orange Book, p. 172

supramolecular chemistry

A field of chemistry related to species of greater complexity than molecules, that are held together and organized by means of intermolecular interactions. The objects of supramolecular chemistry are supermolecules and other polymolecular entities that result from the spontaneous association of a large number of components into a specific phase (membranes, vesicles, micelles, solid state structures *etc.*)

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1964

supramolecule

A system of two or more molecular entities held together and organized by means of intermolecular (noncovalent) binding interactions.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169

surface

The boundary between two phases. It is recommended that for the purpose of surface analysis a distinction be made between 'surface' in general, 'physical surface' and 'experimental surface': Surface — The 'outer portion' of a sample of undefined depth; to be used in general discussions of the outside regions of the sample. Physical Surface — That atomic layer of a sample which, if the sample were placed in a vacuum, is the layer 'in contact with' the vacuum; the outermost atomic layer of a sample. Experimental Surface — That portion of the sample with which there is significant interaction with the particles or radiation used for excitation. It is the volume of sample required for analysis or the volume corresponding to the escape for the emitted radiation or particle, whichever is larger.
See also: interface

Source:
Orange Book, p. 251
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2246

surface amount, n^{s}, n^{a}

Amount of substance adsorbed on a surface.

Source:
Green Book, 2nd ed., p. 63

surface barrier semiconductor detector

A semiconductor detector utilizing a junction due to a surface inversion layer.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1552

surface catalysis

See: homogeneous catalysis

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 763

surface charge density, σ

Electric charge on a surface divided by the surface area.

Source:
Green Book, 2nd ed., p. 14

surface chemical potential

Defined by:

$$\mu_i^{\sigma} = \left(\frac{\partial A^{\sigma}}{\partial n_i^{\sigma}}\right)_{T,A_{\mathrm{S}},n_j^{\sigma}} = \left(\frac{\partial G^{\sigma}}{\partial n_i^{\sigma}}\right)_{T,p,\gamma,n_j^{\sigma}}$$

$$\mu_i^{\mathrm{S}} = \left(\frac{\partial A^{\mathrm{S}}}{\partial n_i^{\mathrm{S}}}\right)_{T,V^{\mathrm{S}},A_{\mathrm{S}},n_j^{\mathrm{S}}} = \left(\frac{\partial G^{\mathrm{S}}}{\partial n_i^{\mathrm{S}}}\right)_{T,p,\gamma,n_j^{\mathrm{S}}}$$

where A^{σ} is the surface excess Helmholtz energy, G^{σ} is the surface excess Gibbs energy A^{S} is the interfacial Helmholtz energy, G^{S} is the interfacial Gibbs energy, and A_{S} is the surface area. The quantities thus defined can be shown to be identical, and the conditions of equilibrium of component i in the system to be

$$\mu_i^{\alpha} = \mu_i^{\sigma} = \mu_i^{\mathrm{S}} = \mu_i^{\beta}$$

where μ_i^{α} and μ_i^{β} are the chemical potentials of i in the bulk phases α and β. (μ_i^{α} or μ_i^{β} have to be omitted from this equlibrium condition if component i is not present in the respective bulk phase.) The surface chemical potentials are related to the Gibbs energy functions by the equations

$$G^{\sigma} = \sum_i n_i^{\sigma}\, \mu_i^{\sigma}$$

$$G^{\mathrm{S}} = \sum_i n_i^{\mathrm{S}}\, \mu_i^{\mathrm{S}}$$

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 602

surface concentration, Γ

Amount of substance adsorbed on a surface divided by the surface area.
See: concentration in experimental surface

Source:
Green Book, 2nd ed., p. 42

surface contamination

in surface analysis

Material in the experimental surface which is either not characteristic of the sample or which would not be present if the sample had been prepared in an absolute vacuum by methods not contacting other substances to the sample.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

surface coverage, θ

Number of adsorbed molecules on a surface divided by the number of molecules in a filled monolayer on that surface.

Source:
Green Book, 2nd ed., p. 63
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2247

surface crossing

In a diagram of electronic energy versus molecular geometry, the electronic energies of two states of different symmetry may be equal at certain geometrical parameters. At this point (unidimensional representation), line or surface (more than one dimension), the two potential-energy surfaces are said to cross one another.
See: avoided crossing

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2279

surface density, ρ_A, ρ_S

Mass divided by area.

Source:
Green Book, 2nd ed., p. 12
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 994

surface dipole layer

Also contains definition of: surface potential

Particles in the surface region of a phase are subjected to orienting forces as a result of the anisotropic force field. Polar molecules (e.g. permanent dipoles) may thus be preferentially oriented in the surface region, while polarizable molecules may be polarized (induced dipoles). The array of oriented polar and/or polarized molecules is called the surface dipole layer with which an electric potential drop is associated, called the surface potential of the phase.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1254

surface electric potential

Given by

$$\chi^{\beta} = \Phi^{\beta} - \psi^{\beta}$$

where ψ^{β} and Φ^{β} are the outer and inner electric potentials of phase β, respectively.

Source:
PAC, 1974, *37*, 499 *(Electrochemical nomenclature)* on page 506
Green Book, 2nd ed., p. 59

surface excess, n^{σ}

For an interface, the adsorption or surface excess of a given component is defined as the difference between the amount of component actually present in the system, and that which would be present (in a reference system) if the bulk concentration in the adjoining phases were maintained up to a chosen geometrical dividing surface (Gibbs dividing surface). For a solid/liquid interface in which no component of the liquid phase penetrates into the solid, the surface excess (or adsorption) of component *i* is defined as:

$$n_i^{\sigma} = n_i - V^{1} c_i^{1}$$

where n_i is the total amount of *i* in the system, V^{1} is the volume of an arbitrarily chosen amount of bulk liquid (in the framework of the so-called algebraic method) and c_i^{1} is its bulk concentration in the liquid.
See: Gibbs adsorption

Source:
PAC, 1986, *58*, 967 *(Reporting data on adsorption from solution at the solid/solution interface (Recommendations 1986))* on page 969
Green Book, 2nd ed., p. 63

surface excess concentration (at an interface), Γ

A quantity defined by

$$\Gamma_i = \frac{n_i^{\sigma}}{A_{\mathrm{s}}}$$

where n_i^{σ} is the surface excess (or adsorption) of component i and A_{s} is the area of the dividing surface or interface.

Source:
PAC, 1986, *58*, 967 *(Reporting data on adsorption from solution at the solid/solution interface (Recommendations 1986))* on page 970
Green Book, 2nd ed., p. 63

surface (excess) conductivity

The excess conductivity in a surface per unit length and width, symbol κ^{σ}.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 621

surface excess energy

Defined by:

$$U^{\sigma} = U - U^{\alpha} - U^{\beta} = U - V^{\alpha}\,\frac{U_{\mathrm{m}}^{\alpha}}{V_{\mathrm{m}}^{\alpha}} - V^{\beta}\,\frac{U_{\mathrm{m}}^{\beta}}{V_{\mathrm{m}}^{\beta}}$$

where V^{α} and V^{β} satisfy the condition $V^{\alpha} + V^{\beta} = V$, the total volume of the system. $(\frac{U_{\mathrm{m}}^{\alpha}}{V_{\mathrm{m}}^{\alpha}})$ and $(\frac{U_{\mathrm{m}}^{\beta}}{V_{\mathrm{m}}^{\beta}})$ are the energy densities in the two bulk phases where U_{m}^{α} and U_{m}^{β} are the mean molar energies and V_{m}^{α} and V_{m}^{β} are the mean molar volumes of the two phases.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 599

surface excess enthalpy

Defined by:

$$H^{\sigma} = U^{\sigma} - \gamma\,A_{\mathrm{s}}$$

where U^{σ} is the surface excess energy, γ is the surface tension, and A_{s} is the area relative to a Gibbs surface.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 599

surface excess entropy

Defined by:

$$S^{\sigma} = S - S^{\alpha} - S^{\beta} = S - V^{\alpha}\,\frac{S_{\mathrm{m}}^{\alpha}}{V_{\mathrm{m}}^{\alpha}} - V^{\beta}\,\frac{S_{\mathrm{m}}^{\beta}}{V_{\mathrm{m}}^{\beta}}$$

$(\frac{S_{\mathrm{m}}^{\alpha}}{V_{\mathrm{m}}^{\alpha}})$ and $(\frac{S_{\mathrm{m}}^{\beta}}{V_{\mathrm{m}}^{\beta}})$ are the entropy densities in the two bulk phases, where S_{m}^{α} and S_{m}^{β} are the mean molar entropies and V_{m}^{α} and V_{m}^{β} are the mean molar volumes of the two phases.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 599

surface excess Gibbs energy

Defined by

$$G^{\sigma} = H^{\sigma} - T\,S^{\sigma} = A^{\sigma} - \gamma\,A_{\mathrm{s}}$$

where H^{σ} is the surface excess enthalpy, T is the thermodynamic temperature, S^{σ} is the surface excess entropy, A^{σ} is the surface excess Helmholtz energy, γ is the surface tension, and A_{s} is the area relative to a Gibbs surface.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 599

surface excess Helmholtz energy

Defined by:

$$A^{\sigma} = U^{\sigma} - T\,S^{\sigma}$$

where U^{σ} is the surface excess energy, T is the thermodynamic temperature, and S^{σ} is the surface excess entropy.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 599

surface excess isotherm

The function relating, at constant temperature and pressure, $\mathit{\Gamma}_i^{(\mathrm{n})}$, $\mathit{\Gamma}_i^{(1)}$ or $\mathit{\Gamma}_i^{(\mathrm{v})}$, or the respective specific quantities $\frac{n^{1}\,\Delta x_i^{1}}{m}$, $\frac{A_{\mathrm{s}}\,\mathit{\Gamma}_i^{(1)}}{m}$ or $\frac{V^{1}\,\Delta c_i^{1}}{m}$ to the mole fraction (or concentration) of component i in the equilibrium liquid phase. With solutions of more than two components such isotherms are unequivocal functions only when the ratios of the mole fractions (or concentrations) of all other components except i are kept constant. (A_{s} is the area of interface, $\mathit{\Gamma}_i^{(\mathrm{n})}$, $\mathit{\Gamma}_i^{(1)}$, $\mathit{\Gamma}_i^{(\mathrm{v})}$ are relative adsorptions, Δx_i^{1} is the change in mole fraction of i resulting from bringing a specified mass m of solid into contact with a specified amount of solution n^{1}, Δc_i^{1} is the change in concentration resulting from bringing a specified mass of solid into contact with a specified amount of solution of volume V^{1}.)

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 593

surface grafting

Process in which a polymer surface is chemically modified by grafting or by the generation of active sites that can lead to the initiation of a graft polymerization.
Notes:

1. Peroxidation, ozonolysis, high-energy irradiation, and plasma etching are methods of generating active sites on a polymer surface.
2. ***See also:*** grafting.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 895

surface ionization

in mass spectrometry

Takes place when an atom or molecule is ionized when it interacts with a solid surface. Ionization occurs only when the work function of the surface, the temperature of the surface, and the ionization energy of the atom or molecule have an appropriate relationship.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548

surface ions

Ions that are constituents of the surface or which have a particularly high affinity for the surface or surface sites.

Source:
PAC, 1991, *63*, 895 *(Nomenclature, symbols, definitions and measurements for electrified interfaces in aqueous dispersions of solids (Recommendations 1991))* on page 899

surface layer (or interfacial layer)

The region of space comprising and adjoining the phase boundary within which the properties of matter are significantly different from the values in the adjoining bulk phases.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 583

surface of a phase (free surface)

The plane ideally marking the boundary between a phase and its environment.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1252

surface of tension

The mechanical properties of an interfacial layer between two fluid phases may be expressed in terms of those of a geometrical surface of uniform tension called the surface of tension, whose location is dependent on the distribution of the stress tensor within the interfacial layer.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 596

surface pressure

The change of interfacial tension caused by addition of a given species to a base solution. When an area of liquid covered with a spread substance is separated from a clean area of surface by a mechanical barrier, the force acting on unit length of the barrier is called the surface pressure, π or π_{s}, and is equal to $\gamma^0 - \gamma$ where γ^0 is the surface tension of the clean surface and γ that of the covered surface.

Source:
PAC, 1972, *31*, 49 *(Extended chain crystals of linear high polymers)* on page 59
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1264
Green Book, 2nd ed., p. 63

surface region

The tridimensional region, extending from the free surface of a condensed phase towards the interior, where the properties differ from the bulk. The term surface may also be used in this sense.

Source:
PAC, 1983, *55*, 1251 *(Interphases in systems of conducting phases (Provisional))* on page 1253

surface shear viscosity

Also contains definitions of: area viscosity, surface dilatational viscosity

For steady state deformations a surface shear viscosity η^{s}, and an area viscosity or surface dilatational viscosity ζ^{s} can be defined. In a Cartesian system with the x-axis normal to the surface, they are defined by the equations:

$$\eta^{\mathrm{s}} = \frac{\sigma_{xy}}{\frac{\partial v_y}{\partial v_x}}$$

$$\zeta^{\mathrm{s}} = \frac{\Delta\gamma}{\frac{\mathrm{d}(\ln A)}{\mathrm{d}t}}$$

where σ_{xy} is the shear component of the surface stress tensor, v_x and v_y are the x and y components of the surface velocity vector, respectively, A is the surface area, t is the time, and $\Delta\gamma$ is the difference between the (steady state) dynamic surface tension and the equilibrium surface tension.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1218

surface states

Energy levels localized in the surface region of semiconductors, which do not bear any direct relation to the bulk energy distribution, but which can exchange electrons with the bulk. In such a case a space charge may arise even when σ (the free charge density) is zero, i.e. $\sigma = \sigma_{\mathrm{sc}} + \sigma_{\mathrm{ss}}$, where σ_{sc} is the space charge density and σ_{ss} is the charge density associated with the surface states.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 443

surface stress, T_{ij}

The work required to form unit area of new surface by stretching under equilibrium conditions. It is numerically equal to the force acting in the *j*th direction per unit length of exposed edge, the edge being normal to the *i*th direction, that must be applied to a terminating surface to keep it in equilibrium, the *i*th and *j*th directions lying in the plane of the surface.

Source:
PAC, 1986, *58*, 437 *(Interphases in systems of conducting phases (Recommendations 1985))* on page 451

surface tension, γ, σ

Work required to increase a surface area divided by that area. When two phases are studied it is often called interfacial tension.

Source:
Green Book, 2nd ed., p. 12
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 995

surface work

Surface tension is the intensive factor in the differential expression for the work required to increase the area of the surface of tension. Measured under reversible conditions at constant temperature (and normally constant pressure) and referred to unit area, this work, the so-called (differential) surface work, is equal to the static surface tension.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 597

surfactant (surface active agent)

A substance which lowers the surface tension of the medium in which it is dissolved, and/or the interfacial tension with other phases, and, accordingly, is positively adsorbed at the liquid/vapour and/or at other interfaces.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 611

surprisal analysis

The study of product state distributions in terms of surprisals has been referred to as surprisal analysis.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 188

surprisal, s

A function relating the prior distribution P_0 of product states to an observed or calculated product distribution P. It is defined by:

$$s = -\ln\left(\frac{P}{P_0}\right).$$

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 188

suspended matter

in atmospheric chemistry

All particulate material which persists in the atmosphere or in a flue gas stream for lengthy periods because the particles are too small in size to have an appreciable falling velocity.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2217

suspension

A liquid in which solid particles are dispersed.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 606

suspension effect

in an ion-selective electrode

An effect which occurs when ion-selective electrodes are used in concentrated, space-filled suspensions while the external reference electrode remains in the supernatant (suspension-free) solution. The suspensions are specifically solvent-swollen ion exchangers or other materials, like soils and clays, that concentrate ions by adsorption and absorption. Space-filled, gravity-packed suspensions act like a second phase and form apparently an interfacial potential difference (PD) with respect to the supernatant. The measured ion activity in the suspension differs from the value in the supernatant by the interfacial PD, and corresponds to a higher value approximating the activity inside the ion exchanger gel. The effect nearly disappears when the outer reference electrode is placed in the same region of the suspension as the sensor electrode. There are some changes in the junction potential differences of the reference electrode, between suspension and supernatant.

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2533

Swain–Lupton equation

A dual parameter approach to the correlation analysis of substituent effects, which involves a field constant (F) and a resonance constant (R). The original treatment was modified later. The procedure has been considerably applied, but also much criticized.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1170

Swain–Scott equation

The linear free-energy relation of the form:

$$\log_{10}\left(\frac{k}{k_0}\right) = s\,n$$

applied to the variation of reactivity of a given electrophilic substrate towards a series of nucleophilic reagents. n is characteristic of the reagent (i.e. a measure of its nucleophilicity) and s is characteristic of the substrate (i.e. a measure of its sensitivity to the nucleophilicity of the reagent). A scale of n values is based on the rate coefficients k for the reaction of methyl bromide with nucleophiles in water at 25 °C, s being defined as 1.00 for these reactions and n being defined as 0.00 for the hydrolysis of methyl bromide. (Other scales have been devised.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1169

swelling agent

Fluid used to swell a gel, network or solid.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1809

swelling

in colloid and surface chemistry

The increase in volume of a gel or solid associated with the uptake of a liquid or gas.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 615

swelling pressure

in colloid and surface chemistry

That pressure difference Π_{sw} or Π which has to be established between a gel and its equilibrium liquid, to prevent further swelling of the gel.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 615

switchboard model

in polymer crystals

A model of crystallinity in which the crystallized segments of a macromolecule belong to the same crystal, although the stems are connected randomly.

Source:
Purple Book, p. 84

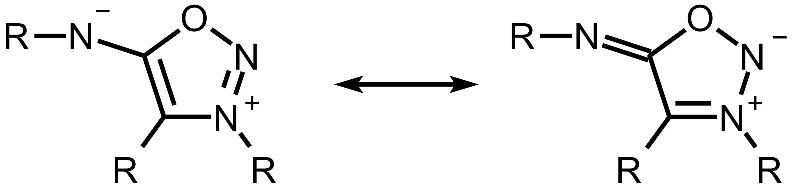
switching transition

A transition in semiconductive glasses in which, beyond a critical applied voltage, there is an avalanche breakdown of conducting electrons that causes local melting and hence local crystallization that gives metallic conductivity.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 592

sydnone imines

Imines of sydnones (i.e. having an imino group in place of the exocyclic oxygen atom).

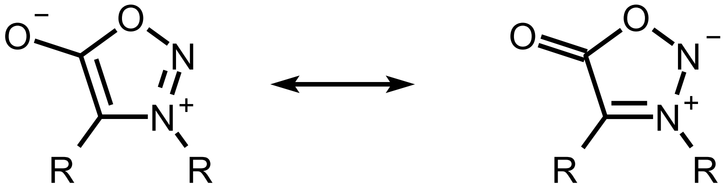


(These structures represent only two canonical forms.)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

sydnones

Mesoionic compounds having the 1,2,3-oxadiazole skeleton bearing an oxygen atom attached to the 5 position.



(These structures represent only two canonical forms).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1370

sym-

An affix used in names to denote symmetrical.

Source:
Red Book, p. 245
Blue Book, p. 465

symbiosis

The term was originally applied to describe the maximum flocking of either hard or soft ligands in the same complexes. For hydrocarbon molecules, symbiosis implies that those containing a maximum number of C–H bonds (e.g. CH_4) or C–C bonds (e.g. Me_4C) are the most stable.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1170

symbol

in quantities and units

Conventional sign designating a quantity or a unit of measurement.
Notes:

1. Symbols for quantities are denoted by letters of the Latin or Greek alphabet printed in italic (sloping) type; pH is an exception.
2. Symbols for units are denoted by letters of the Latin or Greek alphabet printed in roman (upright) type.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 995

symmetrical films

Also contains definition of: unsymmetrical films

The properties of fluid films depend on the nature of the film phase and that of each of the two neighbouring bulk phases. These films should be described, where appropriate, by three capital letters such as A for air, W for water, O for oil, and S for solid, separated by solidi, the middle letter indicating the film phase. For symmetrical films the first and last symbols are the same, e.g. A/W/A: water film in air, or W/O/W: oil film in water, whereas for unsymmetrical films these are different, e.g. W/O/A: oil film between water and air.
See also: asymmetric film

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 613

symmetry number, s

The symmetry number of a molecule is obtained by imagining all identical atoms to be labelled, and then counting the number of different but equivalent arrangements that can be obtained by rotating (but not reflecting) the molecule. In the statistical-mechanical treatment of chemical equilibrium, the partition function for each molecular species must be divided by its symmetry number.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 189
Green Book, 2nd ed., p. 40

symmetry-breaking transition

See: subgroup-supergroup transition

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 592

symmetry-conserving transition

A transition in which the cell dimensions and/or angles of the one phase differ from those in the other phase, but where the space-group symmetry is conserved. Example: The transition of face-centred cubic Ce, upon cooling, to a face-centred cubic phase that is 10% denser. Upon cooling, enough contraction takes place to allow an overlap of the fsp^2 configuration and the change from an isolated non-bonding magnetic f electron to a bonding non-magnetic electron pair.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 592

symproportionation

Synonymous with comproportionation.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1170

syn

1. ***See:*** torsion angle
2. ***See:*** *endo*, *exo*, *syn*, *anti*
3. ***See:*** *anti*
4. Formerly used to describe the stereochemistry of oximes and related systems.
   See: *E*,*Z*

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2220

synchronization (principle of nonperfect synchronization)

This principle applies to reactions in which there is a lack of synchronization between bond formation or bond rupture and other primitive changes that affect the stability of products and reactants, such as resonance, solvation, electrostatic, hydrogen bonding and polarizability effects. The principle states that a product-stabilizing factor whose development lags behind bond changes at the *transition state*, or a reactant-stabilizing factor whose loss is ahead of bond changes at the transition state, increases the intrinsic barrier and decreases the 'intrinsic rate constant' of a reaction. For a product-stabilizing factor whose development is ahead of bond changes, or reactant factors whose loss lags behind bond changes, the opposite relations hold. The reverse effects are observable for factors that destabilize a reactant or product.
See also: imbalance, synchronous

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1170

synchronous

A concerted process in which the primitive changes concerned (generally bond rupture and bond formation) have progressed to the same extent at the transition state is said to be synchronous. The term figuratively implies a more or less synchronized progress of the changes. However, the progress of the bonding change (or other primitive change) has not been defined quantitatively in terms of a single parameter applicable to different bonds or different bonding changes. The concept is therefore in general only qualitatively descriptive and does not admit an exact definition except in the case of concerted processes involving changes in two identical bonds.
See also: imbalance

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1170

synchronously excited (fluorescence, phosphorescence) spectrum

A two-dimensional spectrum obtained by varying both the excitation and emission wavelengths simultaneously and which corresponds to the curve where a plane, parallel to the z-axis, intersects the excitation-emission spectrum (EES).

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 242

synchrotron radiation

X-Radiation which results from the acceleration of charged particles in circular orbits by strong electric and magnetic fields.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 737

syndet

A synthetic detergent; a detergent other than soap.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 612

syndiotactic macromolecule

A tactic macromolecule, essentially comprising alternating enantiomeric configurational base units, which have chiral or prochiral atoms in the main chain in a unique arrangement with respect to their adjacent constitutional units.
Notes:

1. In a syndiotactic macromolecule, the configurational repeating unit consists of two configurational base units that are enantiomeric.
2. A syndiotactic macromolecule consists of racemo diads.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2292

syndiotactic polymer

A polymer composed of syndiotactic macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2302

syndiotactic triads

in polymers

See: triads

Source:
Purple Book, p. 40

syneresis

Spontaneous shrinking of a gel with exudation of liquid.
Note:
Bond formation or attraction between particles or network chains within a gel induces the contraction and thereby the exudation of liquid from the network.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1826

synergism

in solvent extraction

A term describing the co-operative effect of two (or more) extractants where the distribution ratio for the combination is greater than the largest individual distribution ratio (measured under comparable conditions).
Notes:
1. The corresponding adjective is synergic and the term synergistic should not be used.
2. No standard method for quantification of the phenomenon has been agreed and any approach should be clearly defined in a given situation.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2379

synergism

in toxicology

Pharmacological or toxicological interaction in which the combined biological effect of two or more substances is greater than expected on the basis of the simple summation of the toxicity of each of the individual substances.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2103

synoptic scale

In meteorology, the size or scale of ordinary weather systems or cyclones; typically $1000\ \mathrm{km}$ horizontally.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2217

syntectic reaction

A reversible reaction that involves the conversion of two liquid phases, l' and l'', into a solid phase α on cooling:

$$\mathrm{l}' + \mathrm{l}'' \rightleftharpoons \alpha$$

The maximum temperature at which this reaction can occur is the congruent melting point of the solid phase. Example: The conversion of co-existing K-rich and Zn-rich phases in the K-Zn system to form an intermediate solid phase KZn_{13}.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 592

synthetic graphite

A material consisting of graphitic carbon which has been obtained by graphitizing of non-graphitic carbon by chemical vapour deposition (CVD) from hydrobcarbons at temperatures above $2500\ \mathrm{K}$, by decomposition of thermally unstable carbides or by crystallizing from metal melts supersaturated with carbon.
Note:
The term artificial graphite is often used as a synonym for synthetic graphite. The term synthetic graphite is preferred, however, since graphite crystals can be considered to consist of carbon macromolecules. Although the term synthetic graphite also covers the CVD product pyrolytic graphite as well as the residues of carbide decomposition, it is predominantly used for graphitized carbon. Such common use is in line with the above definition. Synonyms for this most important type of synthetic graphite are Acheson graphite and electrographite.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 505

system

Arbitrarily defined part of the universe, regardless of form or size, e.g. for clinical chemistry, patient, patient plasma, patient urine.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 995

system of units

of measurement

Set of base units, together with derived units, defined in accordance with given rules, for a given system of quantities, e.g. Système International d'Unités (SI).

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 995

systematic error

Mean that would result from an infinite number of measurements of the same measurand carried out under repeatability conditions minus a true value of the measurand.

Source:
VIM

See also:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1705
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2188

systematic name

A name composed wholly of specially coined or selected syllables, with or without numerical prefixes; e.g. pentane, oxazole.

Source:
Blue Book, p. xviii

Système International d'Unités

See: SI

Source:
Green Book, 2nd ed., p. 69
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 995

systemic effect

Consequence that is either of a generalized nature or that occurs at a site distant from the point of entry of a substance.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1072

Szilard–Chalmers effect

The rupture of the chemical bond between an atom and the molecule of which the atom is part, as a result of a nuclear reaction of that atom.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

θ state

in polymers

The state of a polymer solution for which the second virial coefficient is zero.
Notes:

1. In some respects, a polymer solution in the θ state resembles an ideal solution and the θ state may be referred to as a pseudo-ideal state. However, a solution in the θ state must not be identified with an ideal solution.
2. The solvent involved is often referred to as 'θ solvent'.
3. It is assumed that the molar mass of the polymer is high.

Source:
Purple Book, p. 57

θ temperature

in polymers

The temperature at which a solution is in the θ state.

Source:
Purple Book, p. 58

tactic block

in a polymer

A regular block that can be described by only one species of configurational repeating unit in a single sequential arrangement.

Source:
Purple Book, p. 17
Purple Book, p. 34

tactic block polymer

A polymer, the molecules of which consist of tactic blocks connected linearly.

Source:
Purple Book, p. 17
Purple Book, p. 34

tactic macromolecule

A regular macromolecule in which essentially all the configurational (repeating) units are identical.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2292

tactic polymer

A polymer composed of tactic macromolecules.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2302

tacticity

The orderliness of the succession of configurational repeating units in the main chain of a regular macromolecule, a regular oligomer molecule, a regular block or a regular chain.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2292

Taft equation

Various equations are associated with R.W. Taft, but the term is most often used to designate the family of equations that emerged from Taft's analysis of the reactivities of aliphatic esters, and which involved the polar substituent constant σ^* and the steric substituent constant E_{s}:

$$\log_{10} k = \log_{10} k_0 + \rho^* \, \sigma^* + \delta \, E_{\mathrm{s}}$$

or the one-parameter forms applicable when the role of either the polar term or the steric term may be neglected. Nowadays σ^* is usually replaced by the related constant σ_I.

See also: Hammett equation, ρ-value, σ-constant

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1171

tagged

Made identifiable by a label.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1553

tailing

in chromatography

Asymmetry of a peak such that, relative to the baseline, the front is steeper than the rear. In paper chromatography and in thin-layer chromatography, the distortion of a zone showing a diffuse region behind the zone in the direction of travel.

Source:
Orange Book, p. 96
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 837

tandem mass spectrometer

An arrangement in which ions are subjected to two or more sequential stages of analysis (which may be separated spatially or temporally) according to the quotient mass/charge. A hybrid mass spectometer is an instrument which combines analysers of different types, e.g. magnetic plus electric sector combined with quadrupole. The study of ions involving two stages of mass analysis has been termed mass spectrometry/mass spectrometry.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

target

in biology

Any organism, organ, tissue, cell, or cell constituent that is subject to the action of an agent.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1072

tautomeric effect [obsolete]

See: electromeric effect

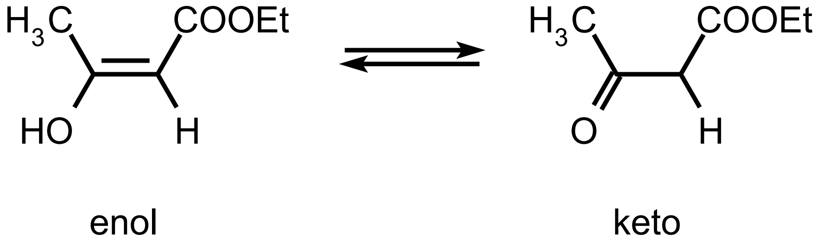
Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1171

tautomerism

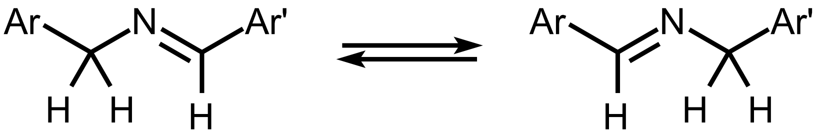
Isomerism of the general form:

$$\mathrm{G{-}X{-}Y{=}Z} \rightleftharpoons \mathrm{X{=}Y{-}Z{-}G}$$

where the isomers (called tautomers) are readily interconvertible; the atoms connecting the groups X, Y, Z are typically any of C, H, O or S, and G is a group which becomes an electrofuge or nucleofuge during isomerization. The commonest case, when the electrofuge is H^+, is also known as 'prototropy'. Examples, written so as to illustrate the general pattern given above, include: Keto-enol tautomerism, such as:

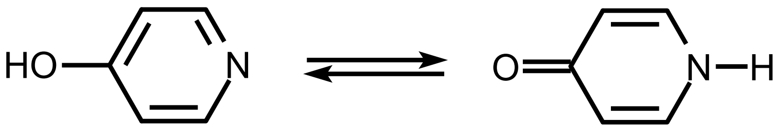


(G = H, X = O, Y= CCH_3, Z = CHCOOEt)



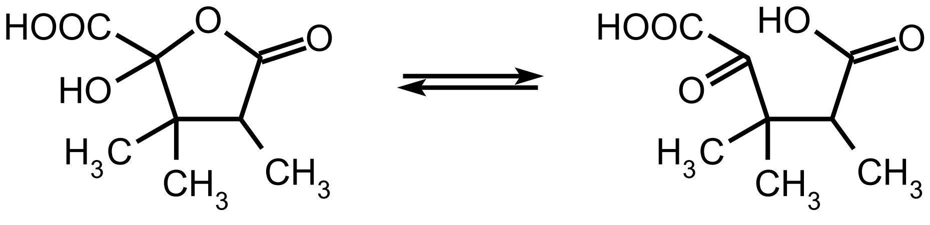
(G = H, X = CHAr, Y = N, Z = CHAr')

The grouping Y may itself be a three-atom (or five-atom) chain extending the conjugation, as in:

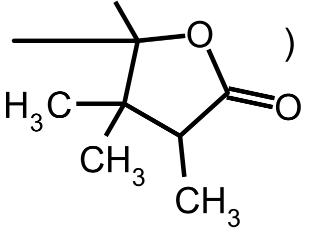


(G = H, X = O, Y = C-CH=CH, Z = N)

The double bond between Y and Z may be replaced by a ring, when the phenomenon is called ring-chain tautomerism, as in:



(G = H, X = O, (Y = Z) =



)

See also: ambident, sigmatropic rearrangement, tautomerization, valence tautomerization

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1171

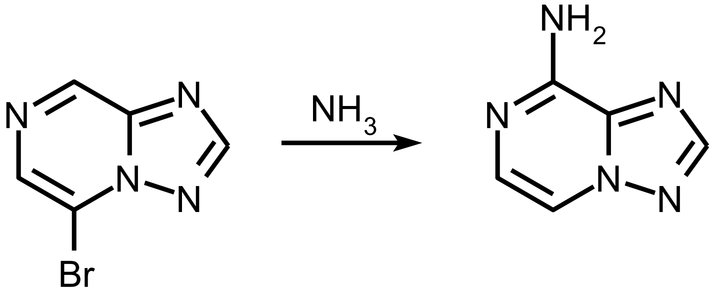
tautomerization

The isomerization by which tautomers are interconverted. It is a heterolytic molecular rearrangement and is frequently very rapid.
See: tautomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1172

tele-substitution

A substitution reaction in which the entering group takes up a position more than one atom away from the atom to which the leaving group was attached:



See also: cine-substitution

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1172

telechelic polymer

Prepolymer capable of entering into further polymerization or other reactions through its reactive end-groups.
Note:
Reactive end-groups in telechelic polymers come from initiator or termination or chain-transfer agents in chain polymerizations, but not from monomer(s) as in polycondensations and polyadditions.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 898

tellurides

1. Compounds having the structure RTeR (R $\neq$ H). Thus tellurium analogues of ethers.
2. Metal salts of tellurane, H_2Te.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

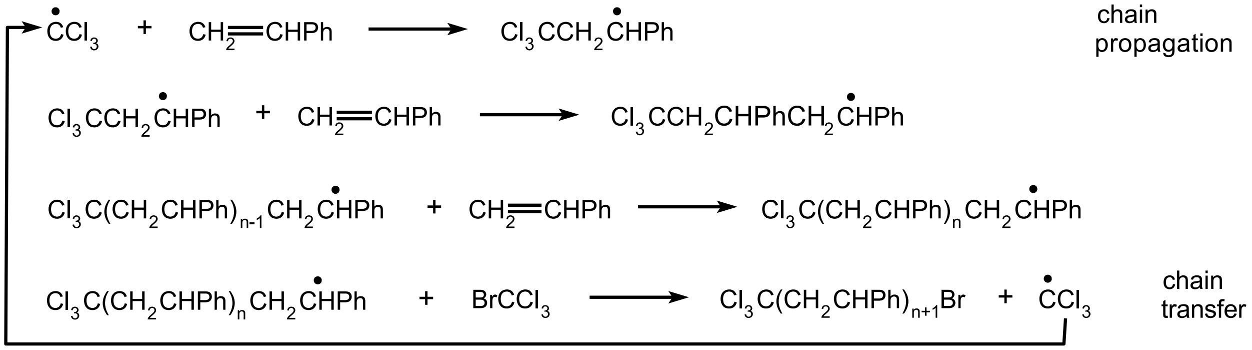
tellurones

Compounds having the structure $R_2Te(=O)_2$. Thus tellurium analogues of sulfones.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

telomerization

The formation of an addition oligomer, having uniform end groups X' ... X" , by a chain reaction in which a chain transfer limits the length of the polymer ('telomer') produced. An example is the polymerization of styrene in bromotrichloromethane solution (X' = CCl_3, X" = Br), where $Cl_3C^{\cdot}$ radicals are formed in the initiation step to produce $Cl_3C[CH_2CHPh]_nBr$, with *n* greater than 1 and often less than *ca*. 10:



See also: oligomerization

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1173

temperature

Short form for thermodynamic, Celsius or Fahrenheit temperature.

Source:
Green Book, 2nd ed., p. 48

temperature coefficient

of responsivity

The dependence of a detector on temperature can be described by the temperature coefficient of responsivity and is expressed as percentage change in output per K. In the case of a nonlinear dependence the temperature and the temperature range should also be stated for which the stated temperature coefficient of responsivity is applicable.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1751

temperature effect

in luminescence spectroscopy

A term used for changes in the luminescence parameters caused by changes in temperature, since the type of solvent and its temperature can effect the luminescence yield from an analyte as a result of quenching, exciplex formation, aggregation, etc.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 244

temperature inversion

in atmospheric chemistry

A departure from the normal decrease of temperature with increasing altitude. A temperature inversion may be produced, for example, by the movement of a warm air mass over a cool one. Intense surface inversions may form over the land during nights with clear skies and low winds due to the radiative loss of heat from the surface of the earth. The temperature increases as a function of height in this case. Poor mixing of the pollutants generally occurs below the inversion, since the normal convective process which drives the warmer and lighter air at ground level to higher altitudes is interrupted as the rising air parcels encounter the warmer air above. Temperature inversions near the surface are particularly effective in trapping ground level emissions.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2197

temperature jump

A relaxation technique in which the temperature of a chemical system is suddenly raised. The system then relaxes to a new state of equilibrium, and analysis of the relaxation processes provides rate constants.
See also: relaxation

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 189

PAC, 1993, *65*, 2291 *(Nomenclature of kinetic methods of analysis (IUPAC Recommendations 1993))* on page 2297

temperature lapse rate

in atmospheric chemistry

The rate of change of temperature with altitude ($\frac{\mathrm{d}T}{\mathrm{d}z}$). The rate of temperature decrease with increase in altitude which is expected to occur in an unperturbed dry air mass is 9.8×10^3 °C min^{-1}. This is called the dry adiabatic lapse rate. The lapse rate is taken as positive when temperature decreases with increasing height. For air saturated with H_2O, the lapse rate is less because of the release of the latent heat of water as it condenses. The average tropospheric lapse rate is about 6.5×10^3 °C min^{-1}. The lapse rate has a negative value within an inversion layer.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2199

temperature-programmed chromatography

A procedure in which the temperature of the column is changed systematically during a part or the whole of the separation.

Source:
Orange Book, p. 92

template

in biotechnology

The nucleic acid single strand that is copied during replication or transcription.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 166

temporary poisoning

in catalysis

Weak and reversible adsorption of a poison, such that removal of the poison from the fluid phase results in restoration of the original catalytic activity.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 83

tera

SI prefix for 10^{12} (symbol: T).

Source:
Green Book, 2nd ed., p. 74

term

in X-ray spectroscopy

A set of levels which have the same electron configuration and the same value of the quantum numbers for total spin S and total orbital angular momentum L.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 737

term symbols

Symbols characterizing the states of atoms and molecules in terms of multiplicity, symmetry of the total electronic wavefunction, and sometimes total (orbital + spin) angular momentum. Examples: $^2\mathrm{P}_{1/2}$ denotes an atomic state of multiplicity 2 (doublet), electron orbital angular momentum quantum number $L = 1$, and orbital plus spin angular momentum quantum number $J = \frac{1}{2}$.

Source:
Green Book, 2nd ed., p. 28

term, *T*

Energy divided by the product of the Planck constant and the speed of light, when of wavenumber dimension, or energy divided by the Planck constant, when of frequency dimension.

Source:
Green Book, 2nd ed., p. 23

termination

The steps in a chain reaction in which reactive intermediates are destroyed or rendered inactive, thus ending the chain.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1173

terminator

in biotechnology

A sequence of DNA lying beyond the 3' end of the coding segment of a gene which is recognized by RNA polymerase as a signal to stop synthesizing mRNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 166

terpenes

Also contains definition of: monoterpenes

Hydrocarbons of biological origin having carbon skeletons formally derived from isoprene [CH_2=C(CH_3)CH=CH_2]. This class is subdivided into the C_5 hemiterpenes, C_{10} monoterpenes, C_{15} sesquiterpenes, C_{20} diterpenes, C_{25} sesterterpenes, C_{30} triterpenes, C_{40} tetraterpenes (carotenoids) and C_{5n} polyterpenes.
See also: carotenes, carotenoids, isoprenoids, prenols, retinoids, steroids, terpenoids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

terpenoids

Natural products and related compounds formally derived from isoprene units (see isoprenoids). They contain oxygen in various functional groups. This class is subdivided according to the number of carbon atoms in the same manner as are terpenes. The skeleton of terpenoids may differ from strict additivity of isoprene units by the loss or shift of a fragment, generally a methyl group.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

See also:
White Book, p. 255

tertiary structure

The spatial organization (including conformation) of an entire protein molecule or other macromolecule consisting of a single chain.
See also: primary structure, secondary structure, quaternary structure

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2220
White Book, p. 80

tesla

SI derived unit of magnetic flux density, $\mathrm{T} = \mathrm{Wb\ m^{-2}} = \mathrm{kg\ s^{-2}\ A^{-1}}$.

Source:
Green Book, 2nd ed., p. 72

test portion

Synonym: analytical portion

The amount or volume of the test sample taken for analysis, usually of known weight or volume.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

See also:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1206

test sample

The sample, prepared from the laboratory sample, from which test portions are removed for testing or for analysis.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1206

See also:
PAC, 1988, *60*, 1461 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-X. Preparation of materials for analytical atomic spectroscopy and other related techniques (Recommendations 1988))* on page 1465

test solution

Synonym: analytical solution

in analysis

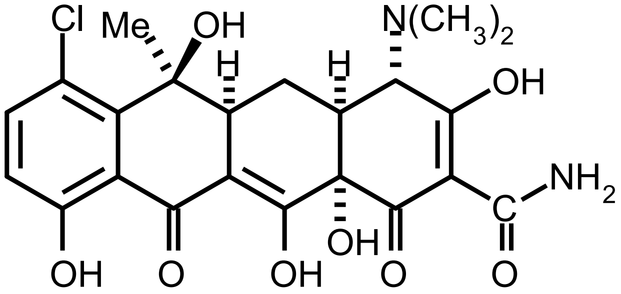
The solution prepared from the test portion for the analytical procedure. The proportions of test portion and solvent are normally known.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1660

See also:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1206

tetracyclines

A subclass of polyketides having an octahydrotetracene-2-carboxamide skeleton, substituted with many hydroxy and other groups, e.g. chlortetracycline:



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

tetrahedral intermediate

A reaction intermediate in which the bond arrangement around an initially double-bonded carbon atom (typically a carbonyl carbon atom) has been transformed from trigonal to tetrahedral. For example, aldol in the condensation reaction of acetaldehyde (but most tetrahedral intermediates have a more fleeting existence).

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1173

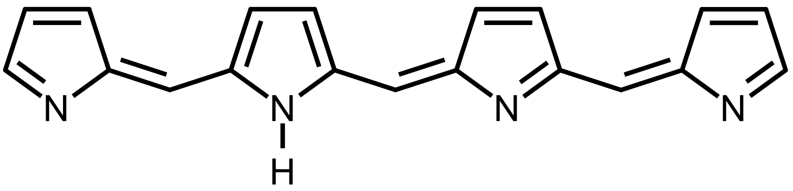
tetrahedro-

An affix used in names to denote four atoms bound into a tetrahedron.

Source:
Red Book, p. 245
Blue Book, p. 465

tetrapyrroles

Natural pigments containing four pyrrole rings joined by one-carbon units linking position 2 of one pyrrole ring to position 5 of the next. Porphyrins are macrocyclic tetrapyrroles. E.g. bilin (a linear tetrapyrrole).



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

See also:
White Book, p. 279

tetraterpenoids

Terpenoids having a C_{40} skeleton.
See also: carotenes, carotenoids, xanthophylls

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

texture

of a catalyst

The detailed geometry of the void space in the particles of a catalyst.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

theoretical ceramic yield

Ceramic yield based on the stoichiometry of the ceramization process.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1810

thermal analysis

A group of techniques in which a physical property of a substance and/or its reaction product is measured as a function of temperature while the substance is subjected to a controlled temperature program.
See also: enthalpimetric analysis

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2488
Orange Book, p. 38

thermal black

A special type of carbon black produced by pyrolysis of gaseous hydrocarbons in a preheated chamber in the absence of air. Thermal black consists of relatively large individual spheres ($100 - 500 \text{ nm}$ diameter) and aggregates of a small number of pseudospherical particles. The preferred alignment of the layer planes is parallel to the surface of the spheres.

Source:
PAC, 1995, *67*, 473 *(Recommended terminology for the description of carbon as a solid (IUPAC Recommendations 1995))* on page 505

thermal column

in nuclear chemistry

A large body of moderator, adjacent to or inside a reactor to provide thermal neutrons for experiments.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1553

thermal conductance, G

Heat flow rate divided by the temperature difference.

Source:
Green Book, 2nd ed., p. 65

thermal conductivity, λ

Tensor quantity relating the heat flux, $\boldsymbol{J}_q$, to the temperature gradient, $\boldsymbol{J}_q = -\lambda \nabla T$.

Source:
Green Book, 2nd ed., p. 37

thermal conductivity detector

in gas chromatography

In general, two cells arranged in a bridge configuration detect the change in thermal conductivity of the gas at the output of the column. This detector is sensitive to any substance with thermal conductivity different from that of the carrier gas. The lowest detectable limit is between 0.5 and 100 ppmv. The linear dynamic range is of the order of 10^3. This type of detector is often used for measuring components at relatively high concentrations.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2192

thermal curing

Curing induced by heating.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1822

thermal fission

Fission caused by thermal neutrons.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1542

thermal ionization

in mass spectrometry

Takes place when an atom or molecule interacts with a heated surface or is in a gaseous environment at high temperature. Examples of the latter may be a capillary arc plasma, a microwave plasma or an inductively coupled plasma.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548
Orange Book, p. 203

thermal lensing

A technique that determines the alteration in the refractive index of a medium as a result of the temperature rise in the path of a laser beam absorbed by the medium. The lens produced (usually divergent) causes a change (usually a decrease) in the irradiance measured along the laser beam axis.
See also: photothermal effects

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2279

thermal neutrons

Neutrons in thermal equilibrium with the medium in which they exist, in general at room temperature.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2522

thermal resistance, *R*

Reciprocal of the thermal conductance.

Source:
Green Book, 2nd ed., p. 65

thermally activated delayed fluorescence

See: delayed fluorescence

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2279

thermally-induced transition

A transition that is induced by a change in temperature. Example: $RbNO_3$ undergoes three structural transitions below 573 K:

1. trigonal → CsCl-type structure at 439 K,
2. CsCl-type → hexagonal structure at 501 K, and
3. hexagonal structure → NaCl-type structure at 551 K.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 592

thermoacoustimetry

A technique in which the characteristics of imposed acoustic waves are measured as a function of temperature after passing through a substance (and/or its reaction product(s)) whilst the substance is subjected to a controlled temperature program.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1740

thermochemical analysis [obsolete]

See: enthalpimetric analysis

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2489

thermochemical calorie

See: calorie

Source:
Green Book, 2nd ed., p. 112
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 996

thermochromism

A thermally induced transformation of a molecular structure or of a system (e.g. of a solution), thermally reversible, that produces a spectral change, typically, but not necessarily, of visible colour.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2279

thermocouple

A device based on the thermoelectric effect, by which two junctions between dissimilar conductors (metallic or heavily doped semiconductors) kept at different temperatures generate an electric potential.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1751

thermodilatometry

A technique in which a dimension of a substance under negligible load is measured as a function of temperature while the substance is subjected to a controlled temperature program. Linear thermodilatometry and volume thermodilatometry are distinguished on the basis of the dimensions measured.

Source:
Orange Book, p. 45

thermodynamic control

Synonym: equilibrium control

of product composition

The term characterizes conditions that lead to reaction products in a proportion governed by the equilibrium constant for their interconversion and/or for the interconversion of reaction intermediates formed in or after the rate-limiting step. (Some workers prefer to describe this phenomenon as 'equilibrium control'.)
See also: kinetic control

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1173

thermodynamic isotope effect

The effect of isotopic substitution on an equilibrium constant is referred to as a thermodynamic (or equilibrium) isotope effect. For example, the effect of isotopic substitution in reactant A that participates in the equilibrium:

$$\mathrm{A} + \mathrm{B} \rightleftharpoons \mathrm{C}$$

is the ratio $\frac{K^{\mathrm{l}}}{K^{\mathrm{h}}}$ of the equilibrium constant for the reaction in which A contains the light isotope to that in which it contains the heavy isotope. The ratio can be expressed as the equilibrium constant for the isotopic exchange reaction:

$$\mathrm{A}^{\mathrm{l}} + \mathrm{C}^{\mathrm{h}} \rightleftharpoons \mathrm{A}^{\mathrm{h}} + \mathrm{C}^{\mathrm{l}}$$

in which reactants such as B that are not isotopically substituted do not appear. The potential energy surfaces of isotopic molecules are identical to a high degree of approximation, so thermodynamic isotope effects can only arise from the effect of isotopic mass on the nuclear motions of the reactants and products, and can be expressed quantitatively in terms of partition function ratios for nuclear motion:

$$\frac{K^{\mathrm{l}}}{K^{\mathrm{h}}} = \frac{\left(Q^{\mathrm{l}}_{\mathrm{nuc}} / Q^{\mathrm{h}}_{\mathrm{nuc}}\right)_{\mathrm{C}}}{\left(Q^{\mathrm{l}}_{\mathrm{nuc}} / Q^{\mathrm{h}}_{\mathrm{nuc}}\right)_{\mathrm{A}}}$$

Although the nuclear partition function is a product of the translational, rotational and vibrational partition functions, the isotope effect is determined almost entirely by the last named, specifically by vibrational modes involving motion of isotopically different atoms. In the case of light atoms (i.e. protium vs. deuterium or tritium) at moderate temperatures, the isotope effect is dominated by zero-point energy differences.
See also: isotopic fractionation factor

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1131

thermodynamic quality of solvent

in polymer chemistry

See: quality of solvent

Source:
Purple Book, p. 57

thermodynamic temperature, *T*

Base quantity in the system of quantities upon which SI is based.

Source:
Green Book, 2nd ed., p. 48
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 996

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2217

thermodynamically equivalent sphere

in polymer chemistry

A sphere, impenetrable to other spheres, displaying the same excluded volume as an actual polymer molecule.

Source:
Purple Book, p. 48

thermoelectrometry

A technique in which an electrical characteristic of a substance (and/or its reaction product(s)) is measured as a function of temperature whilst the substance is subjected to a controlled temperature program. The most common measurements are of resistance, conductance or capacitance.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1740

thermogram **[obsolete]**

See: enthalpogram

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2490

thermogravimetry (TG)

A technique in which the mass of a substance (and/or its reaction product(s)) is measured as a function of temperature whilst the substance is subjected to a controlled temperature program.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1738
Orange Book, p. 39

thermoluminescence

Luminescence arising from a reaction between species trapped in a rigid matrix and released as a result of an increase in temperature.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2279

thermolysis

The uncatalysed cleavage of one or more covalent bonds resulting from exposure of a compound to a raised temperature, or a process in which such cleavage is an essential part.
See also: pyrolysis

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1173

thermomagnetometry

A technique in which a magnetic characteristic of a substance (and/or its reaction product(s)) is measured as a function of temperature whilst the substance is subjected to a controlled temperature program.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1740

thermomechanical measurement

A technique in which the deformation of a substance (and/or its reaction product(s)) under non-oscillatory load is measured as a function of temperature whilst the substance is subjected to a controlled temperature program.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1740

thermometric [obsolete]

See: enthalpimetric analysis, thermometric titration

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2489

thermometric enthalpy titration [obsolete]

See: thermometric titration

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2490

thermometric titration

Synonym: enthalpimetric titration

An analytical method in which one reactant (the titrant) is added continuously or stepwise to an adiabatic or isoperibol vessel containing another reactant. The enthalpy change(s) of the ensuing reaction(s) causes a temperature change which, when plotted versus volume of titrant, may be used to find the titration endpoint(s). This is the preferred term for experiments producing plots of temperature versus volume of titrant in which the main goal is a quantitative determination. Nonetheless, when a calorimetric vessel is used, such that the heat capacity is known, thermodynamic parameters may also be estimated from such experiments. An acceptable synonym in that case is enthalpimetric titration. The use of the adjective thermometric is justified because of widespread historical and current usage, and because a titration of necessity implies a chemical reaction. The term thermometric enthalpy titration has been used, but is not recommended. A method in which the titrant is a catalyst for an indicator reaction that occurs after the endpoint for the analyte reaction should be called a thermometric titration with catalytic endpoint detection, not a catalytic thermometric titration.

Source:
PAC, 1994, *66*, 2487 *(Nomenclature of thermometric and enthalpimetric methods in chemical analysis (IUPAC Recommendations 1994))* on page 2490

thermoparticulate analysis

A thermoanalytical technique in which the release of particulate matter from a substance (and/or its reaction product(s)) is measured as a function of temperature whilst the substance is subjected to a controlled temperature program.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1739

thermophile

An organism that can tolerate high temperatures and that grows optimally at temperatures above 45 °C.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 166

thermopile

Several thermocouples connected in series to increase the magnitude of the electric potential.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1752

thermoplastic elastomer

Elastomer comprising a thermoreversible network.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1811

thermoptometry

Also contains definition of: thermophotometry

A technique in which an optical characteristic of a substance (and/or its reaction product(s)) is measured as a function of temperature whilst the substance is subjected to a controlled temperature program. Measurements of total light, light of specific wavelength(s), refractive index and luminescence lead to thermophotometry, thermospectrometry, thermorefractometry and thermoluminescence, respectively; observation under the microscope leads to thermomicroscopy.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1740

thermoreversible gel

Swollen network in which the junction points are thermally reversible.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1808

thermoreversible junction point

Junction point in a polymer network that can be destroyed and formed reversibly by a change of temperature.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1820

thermoreversible network

Reversible network that forms or breaks up as the temperature is changed.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1815

thermosetting polymer

Prepolymer in a soft solid or viscous state that changes irreversibly into an infusible, insoluble polymer network by curing.
Notes:

1. Curing can be induced by the action of heat or suitable radiation, or both.
2. A cured thermosetting polymer is called a thermoset.

Source:
PAC, 2004, *76*, 889 *(Definitions of terms relating to reactions of polymers and to functional polymeric materials (IUPAC Recommendations 2003))* on page 898

thermosonimetry

A technique in which the sound emitted by a substance (and/or its reaction product(s)) is measured as a function of temperature whilst the substance is subjected to a controlled temperature program.

Source:
PAC, 1985, *57*, 1737 *(Nomenclature for thermal analysis - IV (Recommendations 1985))* on page 1740

thermosphere

Atmospheric shell extending from the top of the mesosphere to outer space. It is a region of more or less steadily increasing temperature with height, starting at 70 or $80\ \mathrm{km}$. It includes the exosphere and most or all of the ionosphere (not the D region).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2217

thermotropic mesophase

A mesophase formed by heating a solid or cooling an isotropic liquid, or by heating or cooling a thermodynamically stable mesophase.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 496

thiazynes

See: hydrocarbylsulfanyl nitrenes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

thickness of diffusion layer

in electrochemistry

The distance from the electrode where the ratio

$$\frac{c - c_{\mathrm{e}}}{c_0 - c_{\mathrm{e}}}$$

reaches a given value. (c_{e} is the interfacial concentration, c is the concentration, c_0 is the value in the bulk solution.) If this ratio is selected as, say, 0.99 the corresponding thickness of the diffusion layer is denoted by $\delta_{0.99}$.
See also: diffusion layer

Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1837

thickness of electrical double layer

The length characterizing the decrease with distance of the potential in the double layer = characteristic Debye length in the corresponding electrolyte solution = κ^{-1}:

$$\frac{1}{\kappa} = \sqrt{\frac{\varepsilon_{\mathrm{r}}\,\varepsilon_0\,R\,T}{F^2 \sum_i c_i\,z_i^2}}$$

(rationalized four-quantity system)

$$\frac{1}{\kappa} = \sqrt{\frac{\varepsilon_{\mathrm{r}}\,R\,T}{4\,\pi\,F^2 \sum_i c_i\,z_i^2}}$$

(three-quantity electrostatic system)

where ε = static permittivity = $\varepsilon_r \, \varepsilon_0$, ε_r = relative static permittivity of solution; ε_0 = permittivity of vacuum, R = gas constant, T = thermodynamic temperature, F = Faraday constant, c_i = concentration of species i, z_i = ionic charge on species i.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 619

thickness of reaction layer

in electrochemistry

When a kinetic current flows, the concentrations of the electroactive substance B and its precursor C at very small distances from the electrode surface are influenced both by mass transfer and by the finite rate of establishment of the chemical equilibrium. As the distance from the electrode surface increases, the chemical equilibrium is more and more nearly attained. The thickness of the reaction layer is the distance from the electrode surface beyond which deviations from the chemical equilibrium between C and B are taken to be negligibly small.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1504

thin film

Also contains definition of: thick film

A film whose thickness is of the order of a characteristic scale or smaller. Since a film may 'look' operationally thin or thick, according to the procedure applied, it is also recommended that the measurement procedure employed be specified (e.g. ellipsometrically thin film, optically thin film, etc.). It is recommended that the physical specification of the film thickness be used, whenever possible (e.g. thick compared to the electron mean free path, thin compared to the optical wavelength, etc.)

Source:
PAC, 1994, *66*, 1667 *(Thin films including layers: terminology in relation to their preparation and characterization (IUPAC Recommendations 1994))* on page 1672

thin-layer chromatography

Chromatography carried out in a layer of adsorbent spread on a support e.g. a glass plate.

Source:
Orange Book, p. 94

thio

This prefix properly denotes replacement of an oxygen by a sulfur, e.g. $PhC(=S)NH_2$, thiobenzamide.

See also entries prefixed thio-.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

thioacetals

Also contains definitions of: dithioacetals, monothioacetals

A term including monothioacetals having the structure $R_2C(OR')(SR')$ (subclass monothioketals, R ≠ H); and dithioacetals having the structure $R_2C(SR')_2$ (subclass dithioketals, R ≠ H, R' ≠ H).
See also: thiohemiacetals

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1371

thioaldehyde *S*-oxides

Compounds having the structure RC(=S=O)H. (Also known by the disapproved term sulfines which includes thioaldehyde *S*-oxides and thioketone *S*-oxides).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thioaldehydes

Compounds in which the oxygen of an aldehyde has been replaced by divalent sulfur, RC(=S)H, e.g. $CH_3CH_2C(=S)H$ propanethial.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thioanhydrides

Synonym: acid thioanhydrides

Compounds having the structure acyl-S-acyl. Also called diacylsulfanes, e.g. $CH_3C(=O)SC(=S)CH_2CH_3$ acetic thiopropanoic thioanhydride.
See: acyl groups

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thiocarboxylic acids

Compounds in which one or both oxygens of a carboxy group have been replaced by divalent sulfur RC(=O)SH or RC(=S)OH monothiocarboxylic acids, RC(=S)SH dithiocarboxylic acids.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thiocyanates

Salts and esters of thiocyanic acid HSC≡N, e.g. $CH_3SC\equiv N$ methyl thiocyanate.
See: isothiocyanates

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thioethers

Former name for sulfides RSR ($R \neq H$).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thiohemiacetals

Compounds of structure $R_2C(SR')OH$ or $R_2C(OR')SH$ (monothiohemiacetals), or $R_2C(SR')SH$ (dithiohemiacetals), $R' \neq H$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thioketone *S*-oxides

Compounds having the structure $R_2C{=}S{=}O$ ($R \neq H$). (Also known by the disapproved term sulfines which comprises thioaldehyde *S*-oxides and thioketone *S*-oxides.)

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thioketones

Compounds in which the oxygen of a ketone has been replaced by divalent sulfur $R_2C{=}S$ ($R \neq H$), e.g. $CH_3C(=S)CH_2CH_3$ butane-2-thione.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thiolates

Derivatives of thiols, in which a metal (or other cation) replaces the hydrogen attached to sulfur, e.g. $CH_3S^-Na^+$ sodium methanethiolate.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

thiols

Compounds having the structure RSH ($R \neq H$), e.g. $MeCH_2SH$ ethanethiol. Also known by the term mercaptans (abandoned by IUPAC).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

third body

A species, other than the reactant itself, which brings about the energization of a molecule that can undergo a unimolecular process, or brings about a combination reaction between atoms or radicals. In the latter case a third body is also called a chaperon.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 189

thixotropic gel

Gel which has a reduced viscosity on the application of a finite shear but which recovers its original viscosity when the shear is discontinued.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1808

thiyl radicals **[obsolete]**

Synonymous with sulfenyl radicals. Due to inconsistencies in use the term is not recommended.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

threshold energy, E_0

Potential energy gap between reactants and the transition state, sometimes involving the zero point energies, but usually not.
See also: critical energy

Source:
Green Book, 2nd ed., p. 56
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 189

threshold limit value (TLV)

The concentration in air to which it is believed that most workers can be exposed daily without an adverse effect (*i.e.*, effectively, the threshold between safe and dangerous concentrations). The values were established (and are revised annually) by the ACGIH and are time-weighted concentrations (TWA) for a 7- or 8-h workday and 40-h workweek, and thus are related to chronic effects. A short-term exposure limit (STEL) is defined as a 15-min TWA exposure, which should not be exceeded at any time during a workday even if the 8-h TWA is within the TLV-TWA.

Source:
PAC, 2001, *73*, 993 *(Risk assessment for occupational exposure to chemicals. A review of current methodology (IUPAC Technical Report))* on page 1024

through-bond electron transfer

Intramolecular electron transfer for which the relevant electronic interaction between the donor and acceptor sites is mediated by through-bond interaction, i.e. via the covalent bonds interconnecting these sites, as opposed to through-space interaction.
See also: through-space electron transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2280

through-space electron transfer

Electron transfer for which the relevant electronic interaction between the donor and acceptor sites is mediated either by direct orbital overlap or by superexchange interaction via intervening molecular entities not covalently bound to the donor or acceptor sites.
See also: through-bond electron transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2280

throughput rate [obsolete]

Usage not recommended.
See: input rate, output rate

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1664

TICT emission

Electronic emission emanating from a TICT state.
See also: twisted internal charge transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2280

TICT state

The acronym derives from Twisted Internal Charge Transfer state, proposed to be responsible for strongly Stokes-shifted fluorescence from certain aromatics, particularly in a polar medium.
See: twisted internal charge transfer

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2280

tie molecule

in polymers

A molecule that connects at least two different crystals.

Source:
Purple Book, p. 83

time, t

Base quantity in the system of quantities upon which SI is based.

Source:
Green Book, 2nd ed., p. 11
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 996

time constant, τ_c

of a detector

If the output of a detector changes exponentially with time, the time required for it to change from its initial value by the fraction $1 - \exp(-t / \tau_c)$ (for $t = \tau_c$) of the final value, is called the time constant.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1751

time, t

of centrifugation

The time difference from switching on until switching off. The time for deceleration is not included.

Source:
PAC, 1994, *66*, 897 *(Quantities and units for centrifugation in the clinical laboratory (IUPAC Recommendations 1994))* on page 905

time of deactivation

in heterogeneous catalysis

See: decay time *in heterogeneous catalysis*

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 83

time

of solidification

of thixotropic recovery

The time in which a certain viscosity or yield stress is reached after discontinuation of a shear. These times depend on the values of viscosity or yield stress chosen by the experimenter.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

time-correlated single photon counting

A technique for the measurement of the time histogram of a sequence of photons with respect to a periodic event, e.g. a flash from a repetitive nanosecond lamp or a CW operated laser (mode locked laser). The essential part is a time-to-amplitude-converter (TAC) which transforms the arrival time between a start and a stop pulse into a voltage. Sometimes called single photon timing.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2280

time-dependent density functional theory

Acronym: TD-DFT

Methods for computing accurate excitation energies at a low computational cost in large molecular species within the time-dependent scheme and the density functional theory. It is the only available DFT-based method for computing electronic excitation energies.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 433

time-dependent stoichiometry

A state in which if intermediates are formed in significant amounts during the course of a reaction, the overall stoichiometric equation does not apply throughout.

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 754

time-independent stoichiometry

A state in which the stoichiometric equation applies throughout the course of the reaction.

Source:
PAC, 1981, *53*, 753 *(Symbolism and terminology in chemical kinetics (Provisional))* on page 754

time-of-flight mass spectrometer

An arrangement using the fact that ions of different mass/charge need different times to travel through a certain distance in a field-free region after they have all been initially given the same translational energy.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546
Orange Book, p. 202

time-resolved fluorometry

See: single-photon timing, frequency-domain fluorometry

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 433

time-resolved microwave conductivity

Acronym: TRMC

Technique allowing the quantitative and qualitative detection of radiation-induced changes in the real, $\Delta\mathrm{Re}\sigma$, and imaginary, $\Delta\mathrm{Im}\sigma$, components of the conductivity of a medium by time-resolved measurement of changes in the microwave absorption resulting from the formation of mobile charges or from changes in the dipole moment or polarizability of molecules on excitation.
Note:
From $\Delta\mathrm{Re}\sigma$ (corresponding to a change in the dielectric loss, $\Delta\varepsilon''$) the product of the yield and the mobility of charges carriers or the dipole moment change can be determined. From $\Delta\mathrm{Im}\sigma$ (corresponding to a change in the relative permittivity, $\Delta\varepsilon'$) the product of the yield and the change in molecular polarizability can be determined.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 433

time-resolved spectroscopy

The recording of spectra at a series of time intervals after the excitation of the system with a light pulse (or other perturbation) of appropriately short duration.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2280

titrant

The solution containing the active agent with which a titration is made.

Source:
Orange Book, p. 47

titration

Also contains definitions of: acidimetric titration, acid–base titration, alkalimetric titration, chelatometric titration, complexometric titration, coulometric titration, equivalence point, precipitation titration

The process of determining the quantity of a substance A by adding measured increments of substance B, with which it reacts (almost always as a standardized solution called the titrant, but also by electrolytic generation, as in coulometric titration) with provision for some means of recognizing (indicating) the endpoint at which essentially all of A has reacted. If the endpoint coincides with the addition of the exact chemical equivalence, it is called the equivalence point or stoichiometric or theoretical endpoint, thus allowing the amount of A to be found from known amounts of B added up to this point, the reacting weight ratio of A to B being known from stoichiometry or otherwise. Terms for varieties of titration can reflect the nature of the reaction between A and B. Thus, there are acid–base, complexometric, chelatometric, oxidation–reduction, and precipitation titrations. Additionally, the term can reflect the nature of the titrant, such as acidimetric, alkalimetric, and iodometric titrations as well as coulometric titrations, in which the titrant is generated electrolytically rather than being added as a standard solution.

Source:
Orange Book, p. 47

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2217

titration curve

A plot of a variable related to a relevant concentration (activity) as the ordinate vs. some measure of the amount of titrant, usually titration volume (titre) as the abscissa. If the variable is linearly related to concentrations, such as the electrical conductance or the photometric absorbance, the term linear titration curve is used. When a logarithmic expression of the concentration or activity is used, such as the pH, pM, or the electrical potential in mV, the curve is referred to as a logarithmic titration curve.

Source:
Orange Book, p. 49

titration error

The difference in the amount of titrant, or the corresponding difference in the amount of substance being titrated, represented by the expression: (end-point value - equivalence-point value).

Source:
Orange Book, p. 48

titre (titer)

The reacting strength of a standard solution, usually expressed as the weight (mass) of the substance equivalent to $1\ \mathrm{cm}^3$ of the solution.

Source:
Orange Book, p. 48

tonne

Non-SI unit of mass, $\mathrm{t} = 10^3\ \mathrm{kg}$.

Source:
Green Book, 2nd ed., p. 111

topical effect

Consequence of application of a substance to the surface of the body which occurs at the point of application.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1073

topochemical reaction

Synonym: topotactic reaction

A reversible or irreversible reaction that involves the introduction of a guest species into a host structure and that results in significant structural modifications to the host, for example, the breakage of bonds. Example: The insertion of lithium at $50\ °C$ into the spinel $Li[Mn_2]O_4$ with symmetry $F\,d3m$ to yield a layered structure with symmetry $P\bar{3}\,m1$.

$$3\ Li + Li[Mn_2]O_4 \longrightarrow 2\ Li_2MnO_2$$

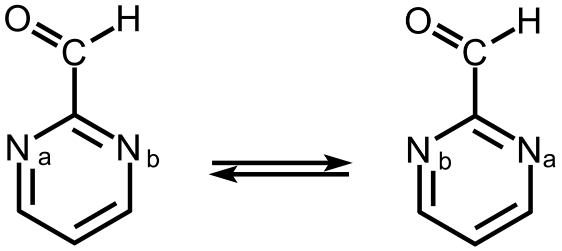
Alternative terms: topotactic reaction, insertion reaction.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 592

topomerization

Also contains definition of: topomers

The identity reaction leading to exchange of the positions of identical ligands. The indistinguishable molecular entities involved are called topomers. For example in the reaction below the two identical ligating atoms N_a and N_b are interchanged by rotation about the C-aryl bond but may be identified by NMR spectroscopy. This is a degenerate isomerization.



Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2220

topotactic transition

A transition in which the crystal lattice of the product phase shows one or more crystallographically equivalent, orientational relationships to the crystal lattice of the parent phase. Example: Transitions in which the anionic array is unchanged during the transition but cation reorganization occurs, as in:

$$\beta\text{-}Li_2ZnSiO_4 \longrightarrow \gamma\text{-}Li_2ZnSiO_4$$

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 593

torque, *T*

Sum of moments of forces not acting along the same line.

Source:
Green Book, 2nd ed., p. 12
ISO 31-2: 1992 *(Quantities and Units - Part 2: Periodic and Related Phenomena.)*

torquoselectivity

The preference for 'inward' or 'outward' rotation of substituents in conrotatory or disrotatory electrocyclic ring opening reactions.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1173

torr

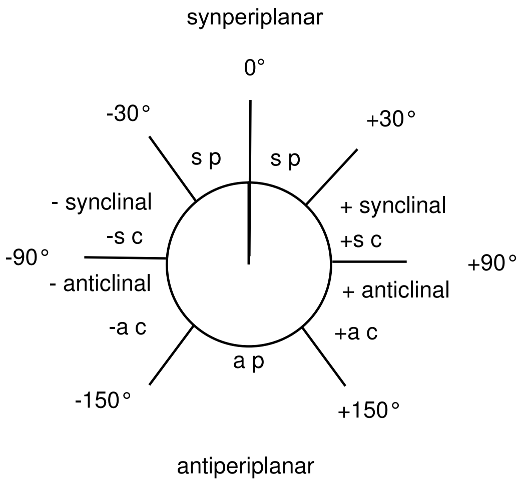
Non-SI unit of pressure, $\text{torr} \approx 133.322\ \text{Pa}$.

Source:
Green Book, 2nd ed., p. 112
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 996

torsion angle

Also contains definitions of: anticlinal, antiperiplanar, clinal, periplanar, synclinal, synperiplanar

In a chain of atoms A-B-C-D, the dihedral angle between the plane containing the atoms A,B,C and that containing B,C,D. In a Newman projection the torsion angle is the angle (having an absolute value between 0° and 180°) between bonds to two specified (fiducial) groups, one from the atom nearer (proximal) to the observer and the other from the further (distal) atom. The torsion angle between groups A and D is then considered to be positive if the bond A-B is rotated in a clockwise direction through less than 180° in order that it may eclipse the bond C-D: a negative torsion angle requires rotation in the opposite sense. Stereochemical arrangements corresponding to torsion angles between 0° and ±90° are called syn (*s*), those corresponding to torsion angles between ±90° and 180° anti (*a*). Similarly, arrangements corresponding to torsion angles between 30° and 150° or between -30° and -150° are called clinal (*c*) and those between 0° and 30° or 150° and 180° are called periplanar (*p*). The two types of terms can be combined so as to define four ranges of torsion angle; 0° to 30° synperiplanar (*sp*); 30° to 90° and -30° to -90° synclinal (*sc*); 90° to 150°, and -90° to -150° anticlinal (*ac*); ±150° to 180° antiperiplanar (*ap*).



The synperiplanar conformation is also known as the syn- or cis-conformation; antiperiplanar as anti or trans and synclinal as gauche or skew. For macromolecular usage the symbols T, C, G^+, G^-, A^+ and A^- are recommended (*ap*, *sp*, *+sc*, *-sc*, *+ac* and *-ac* respectively).

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2220

torsional braid analysis

A particular case of dynamic thermomechanometry in which the material is supported on a braid.

Source:
Orange Book, p. 45

torsional stereoisomers

Stereoisomers that can be interconverted (actually or conceptually) by torsion about a bond axis. This includes *E,Z*-isomers of alkenes, atropisomers and rotamers.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2221

total chemiflux

See: chemical flux

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1095

total consumption time , t_{tot}

in flame emission and absorption spectrometry

The time necessary to consume the prepared sample completely (in s). It is equal to the volume of the prepared sample divided by the rate of fluid consumption.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1740

total ion current

in mass spectrometry

1. (after mass analysis): The sum of the separate ion currents carried by the different ions contributing to the spectrum (this is sometimes called the reconstructed ion current).
2. (before mass analysis): The sum of all the separate ion currents for ions of the same sign before mass analysis.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1554
Orange Book, p. 206

total radiant power

See: spectral radiant power

Source:
PAC, 1985, *57*, 105 *(Names, symbols, definitions and units of quantities in optical spectroscopy (Recommendations 1984))* on page 112

total retention volume (time), V_{R}, t_{R}

in column chromatography

The volume of mobile phase entering the column between sample injection and the emergence of the peak maximum of the sample component of interest, or the corresponding time. It includes the hold-up volume (time):

$$t_{\mathrm{R}} = \frac{V_{\mathrm{R}}}{F_{\mathrm{c}}}$$

where F_c is the mobile phase flow rate at column temperature.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 841

total velocity of the analyte, ν_{tot}

in capillary electrophoresis

The sum of electrophoretic velocity, ν_{ep}, of an ion and the electroosmotic velocity, ν_{eo}.

$$\nu_{\mathrm{tot}} = \nu_{\mathrm{ep}} + \nu_{\mathrm{eo}}$$

This quantity can be measured experimentally as the effective length of the capillary divided by the migration time ($L_{\mathrm{eff}}/t_{\mathrm{m}}$).
Notes:
1. Depending on the signs and relative magnitudes of these velocities, the total velocity of an analyte can have either the same or the opposite direction to the electro- osmotic velocity.
2. The total velocity is the velocity of the ion measured as a displacement relative to the capillary wall divided by time.

Source:
PAC, 2004, *76*, 443 *(Terminology for analytical capillary electromigration techniques (IUPAC Recommendations 2003))* on page 449

totally porous packing

in chromatography

Packing in which the stationary phase permeates each porous particle.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831

toxicity

1. Capacity to cause injury to a living organism defined with reference to the quantity of substance administered or absorbed, the way in which the substance is administered (inhalation, ingestion,

topical application, injection) and distributed in time (single or repeated doses), the type and severity of injury, the time needed to produce the injury, the nature of the organism(s) affected and other relevant conditions.

2. Adverse effects of a substance on a living organism defined with reference to the quantity of substance administered or absorbed, the way in which the substance is administered (inhalation, ingestion, topical application, injection) and distributed in time (single or repeated doses), the type and severity of injury, the time needed to produce the injury, the nature of the organism(s) affected, and other relevant conditions
3. Measure of incompatibility of a substance with life: this quantity may be expressed as the reciprocal of the absolute value of median lethal dose ($\frac{1}{\mathrm{LD}_{50}}$) or concentration ($\frac{1}{\mathrm{LC}_{50}}$).

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2107

toxicodynamics

Study of toxic actions on living systems, including the reactions with and binding to cell constituents, and the biochemical and physiological consequences of these actions.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2108

toxicokinetics

Process of the uptake of potentially toxic substances by the body, the biotransformation they undergo, the distribution of the substances and their metabolites in the tissues, and the elimination of the substances and their metabolites from the body. Both the amounts and the concentrations of the substances and their metabolites are studied. The term has essentially the same meaning as pharmacokinetics, but the latter term should be restricted to the study of pharmaceutical substances.
See also: pharmacokinetics

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2108

toxicology

Scientific discipline involving the study of the actual or potential danger presented by the harmful effects of substances (poisons) on living organisms and ecosystems, of the relationship of such harmful effects to exposure, and of the mechanisms of action, diagnosis, prevention and treatment of intoxications.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2108

toxin

Poisonous substance produced by a biological organism such as a microbe, animal or plant.

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2109

toxinology

Scientific discipline involving the study of the chemistry, biochemistry, pharmacology and toxicology of toxins.
See also: toxicology

Source:
PAC, 1993, *65*, 2003 *(Glossary for chemists of terms used in toxicology (IUPAC Recommendations 1993))* on page 2109

trace element

Any element having an average concentration of less than about 100 parts per million atoms (ppma) or less than $100\ \frac{\mu g}{g}$.

Source:
PAC, 1979, *51*, 2243 *(General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)* on page 2246

traceability

The property of a result or measurement whereby it can be related to appropriate standards, generally international or national standards, through an unbroken chain of comparisons.

Source:
PAC, 1995, *67*, 1699 *(Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))* on page 1701

tracer

A foreign substance mixed with or attached to a given substance to enable the distribution or location of the latter to be determined subsequently. There are several types of tracers which are used: (i) A physical tracer is one that is attached by physical means to the object being traced; (ii) A chemical tracer is a chemical with properties similar to those of the substance being traced with which it is mixed homogeneously; (iii) An isotopic tracer is a unique isotope, either radioactive or an enriched, uncommon stable isotope, of the element to be traced; (iv) A radioactive tracer is a physical or chemical tracer having radioactivity as its distinctive property which allows detection at small concentrations and hence after large transport distances. The composition of aerosols in the troposphere has been used as a qualitative tracer of air masses. The elemental analyses (determined by neutron activation, X-ray fluorescence, etc.) of the aerosols transported from various sources or source regions sometimes have characteristic patterns which are used to define qualitatively the origin of tropospheric aerosols collected in other geographical regions.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2217
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2525

track detector (nuclear)

A detector which makes the paths of ionizing particles visible, either directly (e.g. cloud chamber) or after suitable treatment (photographic emulsion, polymers).

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1553

track (nuclear)

The path of an ionizing particle as revealed by a track detector.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1553

trajectory

in reaction dynamics

A path taken by a reaction system over potential-energy surface or a diagram or mathematical description that represents that path. A trajectory can also be called a reaction path.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 189

trans-

in inorganic nomenclature

A prefix designating two groups directly across a central atom from each other, i.e. in the polar positions on a sphere, not now generally recommended for precise nomenclature purposes.

Source:
Red Book, p. 245

transannular strain

In medium-sized ring compounds, the strain due to repulsive nonbonded interactions between substituents or hydrogen atoms attached to non-adjacent ring atoms.

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2221

transcription

in biotechnology

The process by which the genetic information encoded in a linear sequence of nucleotides in one strand of DNA is copied into an exactly complementary sequence of RNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 167

transducer

An analytical instrument which provides an output quantity having a given relationship to the input quantity.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1662

transduction

in biotechnology

The transfer of genetic information from one bacterium to another by means of a transducing bacteriophage. When the phage is grown on the first host, a fragment of the host DNA can be incorporated into the phage particles. This foreign DNA can be transferred to the second host upon infection with progeny phage from the first experiment.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 167

transfer

Movement of a component within a system or across its boundary. It may be expressed using different kinds of quantities, e.g rates of change $\frac{\mathrm{d}Q}{\mathrm{d}t}$ or $\frac{\Delta Q}{\Delta t}$. Examples are: mass rate, $\frac{\mathrm{d}m_{\mathrm{B}}}{\mathrm{d}t}$ or $\frac{\Delta m_{\mathrm{B}}}{\Delta t}$; substance rate, $\frac{\mathrm{d}n_{\mathrm{B}}}{\mathrm{d}t}$ or $\frac{\Delta n_{\mathrm{B}}}{\Delta t}$.

Source:
PAC, 1992, *64*, 1569 *(Quantities and units for metabolic processes as a function of time (IUPAC Recommendations 1992))* on page 1573

transfer activity coefficient, γ_{t}

A term used to quantify the difference in the free energy of a solute ion in two different standard states often in two different liquid phases. The relationship is $\Delta_{\mathrm{t}}G^{\circ} = \nu\, R\, T\, \ln\gamma_{\mathrm{t}}$ where $\Delta_{\mathrm{t}}G^{\circ}$ is the transfer Gibbs energy and ν is the number of ions in the solute.
Notes:

1. It should not be confused with the mass transfer coefficient which represents the specific rate of transfer of a species from one phase to another.
2. It does not necessarily imply the physical transfer of a solute between two liquid phases.

See also: partition constant

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2386

transfer

in analysis

The action of moving material between containers, or containers between transport devices. This term is of particular importance in clinical chemistry.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1662

transfer line

Line provided to carry the sample to be analysed from the sample point to the analytical unit without altering the composition of the sample.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2218

transfer RNA (tRNA)

A single-stranded RNA molecule containing about 70-90 nucleotides, folded by intrastrand base pairing into a characteristic secondary ('cloverleaf') structure that carries a specific amino acid and matches it to its corresponding codon on an mRNA during protein synthesis.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 167

transferability

Transferability assumes invariance of properties, associated conceptually with an atom or a fragment present in a variety of molecules. The property, such as electronegativity, nucleophilicity, NMR chemical shift, etc. is held as retaining a similar value in all these occurrences.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1173

transferases

Enzymes that catalyse reactions in which a group is transferred from one compound to another. Groups that are transferred are C, aldehydic or ketonic residues, acyl, glycosyl, alkyl, nitrogenous, phosphorus and sulfurcontaining groups.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 167

transformation

The conversion of a substrate into a particular product, irrespective of reagents or mechanisms involved. For example, the transformation of aniline ($C_6H_5NH_2$) into *N*-phenylacetamide ($C_6H_5NHCOCH_3$) may be effected by use of acetyl chloride or acetic anhydride or ketene. A transformation is distinct from a reaction, the full description of which would state or imply all the reactants and all the products.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1173

transformation

in gene technology

A process for genetic alteration of a cell following incorporation of foreign DNA.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 167

transient (chemical) species

Relating to a short-lived reaction intermediate. It can be defined only in relation to a time scale fixed by the experimental conditions and the limitations of the technique employed in the detection of the intermediate. The term is a relative one. Transient species are sometimes also said to be 'metastable'. However, this latter term should be avoided, because it relates a thermodynamic term to a kinetic

property, although most transients are also thermodynamically unstable with respect to reactants and products.
See also: persistent

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1174

transient crosslink

Crosslink formed by intermolecular or intramolecular interactions that are unstable under the conditions of use of the material formed.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1819

transient junction point

Junction point in a polymer network that exists only for a finite period of time.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1820

transient network

Network that exists only transiently.
Note:
The network structure of a transient polymer network is based on transient junction points or crosslinks arising from interactions between polymer chains.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1816

transient phase (induction period)

This expression relates to the period of time that elapdes prior to the establishment of a steady state. Initially the concentration of a reactive intermediate is zero, and it rises to the steady-state concentration during the transient phase.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 189

transient spectroscopy

A technique for the spectroscopic observation of transient species (excited-state molecular entities or reactive intermediates) generated by a pulse of short duration.
See also: flash photolysis, time-resolved spectroscopy

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2280

transient-stimulated emission pumping

Acronym: TSEP

Transient-spectroscopy technique in which the excited state dynamics is probed via stimulating the molecular species from the photo-excited state (produced by a short pump pulse) back to the ground state by means of a short dump pulse at various pump–dump time delays.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 434

transit time, t_{ts}

in flame emission and absorption spectrometry

The time needed for the component to pass through the observation space (in s). It depends on the geometry of the observation space, the flame temperature and the solute nebulized.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1742

transition

See: n → σ* transition, , π → π* transition, π → σ* transition, , σ → σ* transition

Source:
PAC, 1988, *60*, 1055 *(Glossary of terms used in photochemistry (Recommendations 1988))* on page 1079
PAC, 1988, *60*, 1055 *(Glossary of terms used in photochemistry (Recommendations 1988))* on page 1089
PAC, 1988, *60*, 1055 *(Glossary of terms used in photochemistry (Recommendations 1988))* on page 1099

transition coordinate

The reaction coordinate at the transition state corresponding to a vibration with an imaginary frequency. Motion along it in the two opposite senses leads towards the reactants or towards the products.

Source:
PAC, 1994, *66*, 117 *(Biochemical engineering in biotechnology (Technical Report))* on page 117

transition (dipole) moment

Also contains definition of: electronic transition moment

An electromagnetic wave may induce an oscillating electric moment in a molecule (possibly leading to absorption if the oscillation frequency is equal to the light frequency). The amplitude of this moment is the transition momentbetween the initial (i) and final (f) states (here assumed to be non-degenerate):

$$\boldsymbol{M}_{\mathrm{if}} = \langle \mathrm{f} \mid \boldsymbol{M}_{\mathrm{op}} \mid \mathrm{i} \rangle$$

where $\boldsymbol{M}_{\mathrm{op}}$ is the electric dipole moment operator, a vector operator that is the sum of the position vectors of all charged particles weighted with their charge. The transition moment $\boldsymbol{M}_{\mathrm{if}}$ is a vector in the molecular framework, characterized both by its direction and its probability.
Notes:

1. The absorption probability for linearly polarized light is proportional to the cosine square of the angle between the electric vector of the electromagnetic wave and $\boldsymbol{M}_{\mathrm{if}}$; light absorption will be maximized if they are parallel, and no absorption will occur if they are perpendicular.
2. It is frequently said that a transition is polarized along the direction of its transition moment and this direction is called the polarization direction of the transition.
3. In the case of a doubly degenerate final state f, each of the two components at the same energy has a transition moment and the two moments define a plane. The transition is then said to be polarized in that plane, which also defines its polarization direction(s). This is typically the case for some of the transitions in highly symmetrical molecules.
4. In the case of a vibronic transition, where both the initial and the final states may be characterized by (different) electronic and vibrational states, the Franck–Condon principle is often applied. This approximation separates electronic and nuclear descriptions and allows the transition moment to be written as a product of a purely electronic transition moment and an overlap integral between the two vibrational wavefunctions involved.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 434

transition element

An element whose atom has an incomplete d sub-shell, or which can give rise to cations with an incomplete d sub-shell.

Source:
Red Book, p. 43

transition interval

in titrimetric analysis

The range of concentration over which the eye is able to perceive change in hue, colour intensity, fluorescence or other property of a visual indicator arising from the varying ratio of the two relevant forms of the indicator.

Source:
Orange Book, p. 48

transition polarization

The direction of the transition moment in the molecular framework.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2281

transition species

Any intermediate species in an elementary reaction. An activated complex is an example of a transition species, but the latter term also includes other intermediate species. Transition species have also been called transition states, but there is then danger of confusion with a true activated complex, which is also commonly known as a transition state.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 190

transition state

In theories describing elementary reactions it is usually assumed that there is a transition state of more positive molar Gibbs energy between the reactants and the products through which an assembly of atoms (initially composing the molecular entities of the reactants) must pass on going from reactants to products in either direction. In the formalism of 'transition state theory' the transition state of an elementary reaction is that set of states (each characterized by its own geometry and energy) in which an assembly of atoms, when randomly placed there, would have an equal probability of forming the reactants or of forming the products of that elementary reaction. The transition state is characterized by one and only one imaginary frequency. The assembly of atoms at the transition state has been called an activated complex. (It is not a complex according to the definition in this Compendium.) It may be noted that the calculations of reaction rates by the transition state method and based on calculated potential-energy surfaces refer to the potential energy maximum at the saddle point, as this is the only point for which the requisite separability of transition state coordinates may be assumed. The ratio of the number of assemblies of atoms that pass through to the products to the number of those that reach the saddle point from the reactants can be less than unity, and this fraction is the 'transmission

coefficient' κ. (There are also reactions, such as the gas-phase colligation of simple radicals, that do not require 'activation' and which therefore do not involve a transition state.)
See also: Gibbs energy of activation, Hammond principle, potential energy profile, transition structure, activated complex

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1174

transition state analogue

A substrate designed to mimic the properties or the geometry of the transition state of reaction.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1174

transition state theory

A theory of the rates of elementary reactions which assumes a special type of equilibrium, having an equilibrium constant $K^{\ddagger}$, to exist between reactants and activated complexes. According to this theory the rate constant is given by:

$$k = \frac{k_{\mathrm{B}}\, T}{h}\, K^{\ddagger}$$

where k_B is the Boltzmann constant and h is the Planck constant. The rate constant can also be expressed as:

$$k = \frac{k_{\mathrm{B}}\, T}{h}\, \exp\left(\frac{\Delta^{\ddagger}S^{\circ}}{R}\right) \exp\left(-\frac{\Delta^{\ddagger}H^{\circ}}{R\,T}\right)$$

where $\Delta^{\ddagger}S^{\circ}$, the entropy of activation, is the standard molar change of entropy when the activated complex is formed from reactants and $\Delta^{\ddagger}H^{\circ}$, the enthalpy of activation, is the corresponding standard molar change of enthalpy. The quantities E_a (the energy of activation) and $\Delta^{\ddagger}H^{\circ}$ are not quite the same, the relationship between them depending on the type of reaction. Also:

$$k = \frac{k_{\mathrm{B}}\, T}{h}\, \exp\left(-\frac{\Delta^{\ddagger}G^{\circ}}{R\,T}\right)$$

where $\Delta^{\ddagger}G^{\circ}$, known as the Gibbs energy of activation, is the standard molar Gibbs energy change for the conversion of reactants into activated complex. A plot of standard molar Gibbs energy against a reaction coordinate is known as a Gibbs-energy profile; such plots, unlike potential-energy profiles, are temperature-dependent. In principle the equations above must be multiplied by a transmission coefficient, κ, which is the probability that an activated complex forms a particular set of products rather than reverting to reactants or forming alternative products. It is to be emphasized that $\Delta^{\ddagger}S^{\circ}$,

$\Delta^{\ddagger}H^{\circ}$ and $\Delta^{\ddagger}G^{\circ}$ occurring in the former three equations are not ordinary thermodynamic quantities, since one degree of freedom in the activated complex is ignored. Transition-state theory has also been known as absolute rate theory, and as activated-complex theory, but these terms are no longer recommended.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 190

transition structure

A saddle point on a potential-energy surface. It has one negative force constant in the harmonic force constant matrix.
See also: activated complex, transition state

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1174

transition temperature (for liquid crystals)

The temperature at which the transition from mesophase X to mesophase Y occurs.

Source:
PAC, 2002, *74*, 493 *(Definitions of basic terms relating to polymer liquid crystals(IUPAC Recommendations 2001))* on page 496

transition time

in electroanalytical chemistry

In chronopotentiometry and related techniques, the time that elapses between the instant at which current is applied and the instant at which the concentration of an electroactive substance B at the electrode-solution interface becomes indistinguishable from zero. In experimental practice the latter time is often taken to be the instant at which the rate of variation of the potential of the indicator electrode attains a maximum value.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1504

transition wavenumber, $\tilde{\nu}$

Difference of term values for the corresponding states (upper minus lower).

Source:
Green Book, 2nd ed., p. 23

translation

in biotechnology

The unidirectional process that takes place on the ribosomes whereby the genetic information present in an mRNA is converted into a corresponding sequence of amino acids in a protein.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 167

translational spectroscopy

A technique to investigate the distribution of the velocity of product ions from reactions of ions and neutral species.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1556

transmission

See: transmittance

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 996

transmission coefficient

See: transition state, , transition state theory

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1174
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 190

transmission electron energy loss spectroscopy (TEELS)

Any technique in which an electron transparent specimen is bombarded with a finely focused electron beam and the energy distribution of the transmitted electrons is measured. This energy spectrum contains features corresponding to discrete losses of energy of the transmitted electrons due to excitation of electronic or plasmon states and provides information on the identity (and in some cases) chemical bonding of the elements in the sample.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2025

transmission electron microscopy (TEM)

Any technique in which an electron transparent sample is bombarded with an electron beam and the intensity of the transmitted electrons which is determined by scattering phenomena (electron absorption phenomena) in the interior of the sample is recorded. TEM essentially provides a high resolution image of the microstructure of a thin sample. This technique is often just called electron microscopy. The term transmission electron microscopy is however recommended for the sake of a clear distinction from other electron microscopic techniques.

Source:
PAC, 1983, *55*, 2023 *(Nomenclature, symbols and units recommended for in situ microanalysis (Provisional))* on page 2024

transmission factor

See: transmittance

Source:
Green Book, 2nd ed., p. 32

transmission high energy electron diffraction (THEED)

Also contains definition of: selected area electron diffraction (SAED)

Any technique which is based on the diffraction of high energy electrons ($E_0 = 10 - 200\,\mathrm{keV}$) in crystalline materials and evaluation of the angular distribution of the transmitted electrons. The diffraction pattern represents an image of the reciprocal lattice and therefore contains information about crystal structure. This technique is also often called selected area electron diffraction (SAED). For consistency with other electron diffraction techniques, however, the term THEED is recommended.

Source:
Orange Book, p. 248

transmission

in mass spectrometry

The ratio of the number of ions leaving a region of a mass spectrometer to the number entering that region.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

transmittance, T, τ

Also contains definition of: internal transmittance

The ratio of the transmitted radiant power (P_λ) to that incident on the sample (P_λ^0):

$$T = \frac{P_\lambda}{P_\lambda^0}$$

Internal transmittance refers to energy loss by absorption, whereas the total transmittance is that due to absorption, reflection, scatter, etc.
See: absorbance, attenuance, Beer–Lambert law

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2281
Green Book, 2nd ed., p. 32
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 996

transoid conformation [obsolete]

Usage strongly discouraged.
See: s-*cis*, s-*trans*
See: *cisoid*, for use of *transoid*, as a stereodescriptor

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2221

transport control

See: microscopic diffusion control

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1174

transport

Also contains definitions of: centrifugal flow, discrete transport, pressure flow

in analysis

The action of moving materials within the analytical instrument. Transport can involve any of several means including pressure flow, where the materials are moved by fluid pressure, either continuously or discontinuously; centrifugal flow, where the materials are moved by centrifugal force; spontaneous motion, where the materials are moved due to their intrinsic properties, e.g. diffusion, capillarity; and discrete transport, where materials are enclosed within a moving container.

Source:
PAC, 1989, *61*, 1657 *(Nomenclature for automated and mechanised analysis (Recommendations 1989))* on page 1662

transport interference

in flame spectroscopy

Transport interferences affect the amount of desolvated sample passing through the horizontal flame cross-section per unit time at the observation height. They include factors affecting the rate of liquid consumption, F_1, the efficiency of nebulization, ε_n, and the fraction desolvated β_s. They may be classified as non-specific (and physical).

Source:
Orange Book, p. 170

transport number, t

Of ions B, the current density due to ions B divided by the sum of current densities of all the ions in the electrolyte. ISO recommends the name current fraction of ions B.

Source:
Green Book, 2nd ed., p. 60

transposon

A movable DNA element that can be inserted at new sites into plasmids or chromosomes independently of the host cell recombination system. Prokaryotic transposons can carry genes that confer new phenotypic properties, such as resistance to antibiotics on the host.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 167

transtactic polymer

A tactic polymer in which the main-chain double bonds of the configurational base units are entirely in the *trans*-arrangement.

Source:
Purple Book, p. 33

trapping

The interception of a reactive molecule or reaction intermediate so that it is removed from the system or converted into a more stable form for study or identification.
See also: scavenger

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1174

travel time, t_{tv}

in flame emission and absorption spectrometry

The time needed for the component to be carried from the burner tip to the observation space (in s). Travel time depends on the observation height and the flame rise velocity.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1742

treated solution

in analytical chemistry

The test solution that has been subjected to reaction or separation procedures prior to measurement of some property.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1206

triangulo-

An affix used in names to denote three atoms bound into a triangle.

Source:
Red Book, p. 245
Blue Book, p. 465

triazanes

Triazane, NH_2NHNH_2, and its hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

triazenes

Triazene, $NH_2N{=}NH$, and its hydrocarbyl derivatives.
See also: diazoamino compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1372

triboluminescence

Luminescence resulting from the rubbing together of the surface of certain solids. It can be produced, for example, when solids are crushed.
See: sonoluminescence

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2281

trimethylenemethanes

The diradical $CH_2{=}C(C^{\cdot}H_2)_2$, 2-methylenepropane-1,3-diyl, for which no Kekulé structure can be written, and its hydrocarbyl derivatives.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

trioxides

Organic derivatives of trioxidane, HOOOH, e.g. ROOOR'. When R' = H , the compound is a hydrotrioxide.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

triple point

The point in a one-component system at which the temperature and pressure of three phases are in equilibrium. If there are p possible phases, there are $\frac{p\,!}{(p-3)\,!\;3\,!}$ triple points. Example: In the sulfur system four possible triple points (one metastable) exist for the four phases comprising rhombic S (solid), monoclinic S (solid), S (liquid) and S (vapour).

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 593

triplet state

A state having a total electron spin quantum number of 1.
See: multiplicity

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2281

triplet-triplet absorption

Absorption which takes place with the transition from the lowest triplet state of the molecule to higher triplet states (T → T_n) thus leading to the triplet-triplet absorption spectrum.

Source:
PAC, 1984, *56*, 231 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-Part VI: molecular luminescence spectroscopy)* on page 234

triplet-triplet annihilation

Two atoms or molecular entities both in a triplet state often interact (usually upon collision) to produce one atom or molecular entity in an excited singlet state and another in its ground singlet state. This is often, but not always, followed by delayed fluorescence.
See also: annihilation, spin conservation rule

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2281

triplet-triplet energy transfer

Acronym: TTET

Energy transfer from an electronically excited triplet donor to produce an electronically excited acceptor in its triplet state.
See: spin conservation rule

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2282

triplet-triplet transitions

Electronic transitions in which both the initial and final states are triplet states.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2282

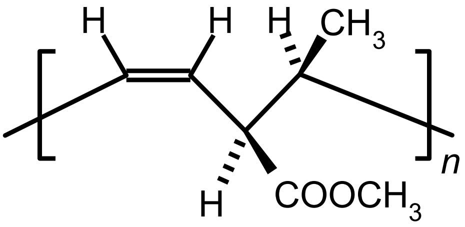
triprismo-

An affix used in names to denote six atoms bound into a triangular prism.

Source:
Red Book, p. 245
Blue Book, p. 465

tritactic polymer

A tactic polymer that contains three sites of defined stereoisomerism in the main chain of the configurational base unit. Example:



Source:
Purple Book, p. 32

triterpenoids

Terpenoids having a C_{30} skeleton.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

tritium

Also contains definitions of: tritide, tritio, triton

A specific name for the atom ^{3}H. The cation $^{3}H^{+}$ is a triton, the species $^{3}H^{-}$ is a tritide anion and ^{3}H is the tritio group.

Source:
PAC, 1988, *60*, 1115 *(Names for hydrogen atoms, ions, and groups, and for reactions involving them (Recommendations 1988))* on page 1116

trivial name

A name having no part used in a systematic sense.

Source:
Blue Book (Guide), p. 14

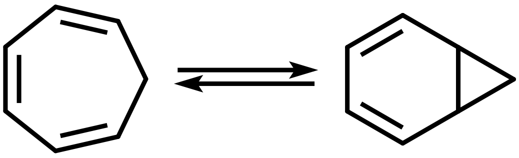
Troe expression

A semiempirical description of the rate coefficient for a specific three body reaction [e.g. $HO + NO_2\ (+\ M) \longrightarrow HONO_2\ (+\ M)$] which represents well its pressure and temperature dependence in the region of transition between second and third order kinetics.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2218

tropilidenes [obsolete]

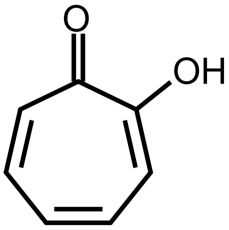
This term has inconsistently been used to mean cyclohepta-1,3,5-trienes or to mean cyclohepta-1,3,5-trienes in dynamic equilibrium with bicyclo-[4.1.0]hepta-2,4-dienes, so that the structure of the bulk substance is indeterminate in the time scale of the method of observation. Use of this term is therefore discouraged.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

tropolones

2-Hydroxycyclohepta-2,4,6-trienones and derivatives formed by substitution.

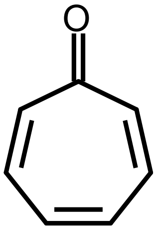


See: tropones

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

tropones

Compounds that contain the cyclohepta-2,4,6-trienone ring system.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

tropopause

The region of the atmosphere which joins the troposphere and stratosphere, and where the decreasing temperature with altitude, characteristic of the troposphere ceases, and the temperature increase with height which is characteristic of the stratosphere begins.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2218

troposphere

The lowest layer of the atmosphere, ranging from the ground to the base of the stratosphere (tropopause) at $10 - 15\ \mathrm{km}$ of altitude depending on the latitude and meteorological conditions. About 70% of the mass of the atmosphere is in the troposphere. This is where most of the weather features occur and where the chemistry of the reactive anthropogenic species released into the atmosphere takes place.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2218

tropyl radicals

The delocalized radicals derived formally by abstraction of one hydrogen from the CH_2 group of cyclohepta-1,3,5-triene and substitution derivatives thereof.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

tropylium ions

The delocalized carbenium ion, cycloheptatrienylium, $C_7H_7^+$, derived formally by detachment of one hydride ion from the CH_2 group of cyclohepta-1,3,5-triene and substitution derivatives thereof.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

true coincidence

in radiochemistry

A coincidence of events occurring in the same atom or in physically connected atoms.

Source:
Orange Book, p. 216

true value, τ

in analysis

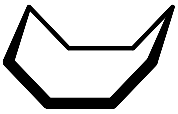
The value that characterizes a quantity perfectly in the conditions that exist when that quantity is considered. It is an ideal value which could be arrived at only if all causes of measurement error were eliminated, and the entire population was sampled.
See also: measurement result

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 598

See also:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 996
VIM

tub conformation

A conformation (of symmetry group D_{2d}) of an eight-membered ring in which the four atoms forming one pair of diametrically opposite bonds in the ring lie in one plane and all other ring atoms lie to one side of that plane. It is analogous to the boat conformation of cyclohexane.



See also: crown conformation

Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2221

tunable laser

in spectrochemical analysis

A high intensity source with narrow spectral bandwidth, with and without frequency doubling and/or Raman shifting. Its use may enable the spectral apparatus to be omitted. Tunable lasers may be either continuous (CW) or pulsed in nature.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1453

Tung distribution

of a macromolecular assembly

A continuous distribution with the differential mass-distribution function of the form:

$$f_{\mathrm{w}}(x)\,\mathrm{d}x = a\,b\,x^{b-1}\,\mathrm{e}^{-a\,x^{b}}\,\mathrm{d}x$$

where x is a parameter characterizing the chain length, such as relative molecular mass or degree of polymerization and a and b are positive adjustable parameters.

Source:
Purple Book, p. 56

tungsten-halogen lamp

tungsten lamp
See: quartz–iodine lamp, wolfram lamp
.
Note:
Halogens other than iodine may fill the lamp.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 436

tunnelling

The process by which a particle or a set of particles crosses a barrier on its potential-energy surface without having the energy required to surmount this barrier. Since the rate of tunnelling decreases with increasing reduced mass, it is significant in the context of isotope effects of hydrogen isotopes.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1174

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2282

turbidimetric titration

The process in which a precipitant is added incrementally to a highly dilute polymer solution and the intensity of light scattered by, or the turbidity due to, the finely dispersed particles of the polymer-rich phase is measured as a function of the amount of precipitant added.

Source:
Purple Book, p. 67

turbidity, τ

in light scattering

The apparent absorbance of the incident radiation due to scattering. For small particles, direct proportionality exists between turbidity and the Rayleigh ratio.

Source:
Purple Book, p. 66

See also:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2218

turnover frequency

in catalysis

Commonly called the turnover number, N, and defined, as in enzyme catalysis, as molecules reacting per active site in unit time.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 81

twisted intramolecular charge transfer

Acronym: TICT

In a TICT state formed by intramolecular charge transfer in an electron donor (D)/acceptor (A) molecule, the D and A subgroups have a mutually perpendicular configuration that leads to electronic decoupling of D and A.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 436

two-dimensional chromatography

A procedure in which parts or all of the separated sample components are subjected to additional separation steps. This can be done e.g. by conducting a particular fraction eluting from the column into another column (system) having different separation characteristics. When combined with additional steps, this may be described as multi-dimensional chromatography. In planar chromatography two-dimensional chromatography refers to the chromatographic process in which the components are caused to migrate first in one direction and subsequently in a direction at right angles to the first one; the two elutions are carried out with different eluents.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 827

two-photon excitation

Excitation resulting from successive or simultaneous absorption of two photons by an atom or molecular entity. This term is used for successive absorption only if some of the excitation energy of the first photon remains in the atom or molecular entity before absorption of the second photon. The simultaneous two-photon absorption can also be called biphotonic excitation.
See: two-photon process

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2282

two-photon photochromism

Photochromic process involving a two-photon process. The process might involve the simultaneous or the sequential absorption of two photons.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 436

two-photon process

A photophysical or photochemical event triggered by a two-photon excitation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2282

two-site immunoradiometric assay

Immunoradiometric assay involving two sets of antibodies, one of which is labelled, that combine with different immunoreactive sites of an antigen molecule.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2520

ultimate capacity

Synonym: stoichiometric capacity

in solvent extraction

The theoretical maximum capacity of a solvent containing a given concentration of extractant for a solute under any conditions. Where appropriate the term stoichiometric capacity can be used.

Source:
PAC, 1993, *65*, 2373 *(Nomenclature for liquid-liquid distribution (solvent extraction) (IUPAC Recommendations 1993))* on page 2386

ultrafiltrate

The solution obtained by ultrafiltration, in general not of the same composition as the equilibrium solution.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 608

ultrafiltration

A separation process whereby a solution containing a solute of molecular size significantly greater than that of the solvent molecule is removed from the solvent by the application of a hydraulic pressure which forces only the solvent to flow through a suitable membrane, usually having a pore size in the range $0.001 - 0.1\ \mu\mathrm{m}$.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 167

ultrasonic detector

in gas chromatography

Sound is generated in a reference cell and a measuring cell. An eluted component passing through the measuring cell changes the velocity of sound in the cell. This change is detected by a phase shift of acoustic signals between the two cells. This detector is usually employed for inorganic gases in the region where thermal conductivity detectors are not sufficiently sensitive. The detection threshold is of the order of $0.1\ \mathrm{ppmv}$. The linear dynamic range is of the order of 10^3.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2192

ultraviolet

Acronym: UV

Region of the electromagnetic spectrum extending from about 100 nm to 400 nm. This region is divided into four sub-bands as follows:

Vacuum Ultraviolet (VUV)	100 nm–200 nm
UV-C	200 nm–280 nm
UV-B	280 nm–315 nm
UV-A	315 nm–400 nm.

Note:
The notation and the limits of the various regions are as recommended by the International Commission on Illumination (CIE), with the exception that in these recommendations the UV-C range is 100 nm–280 nm, including thus the vacuum UV range.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 437

umpire sample

A sample taken, prepared and stored in an agreed upon manner for the purpose of settling a dispute. The agreement usually extends beyond the sample to the basis for reaching a decision (e.g. quantity of material from which taken, use of a third party and criteria serving as the basis for acceptance, rejection or economic adjustment). The term 'reference sample' has been used in this context but this term more properly should be used in conjunction with a 'reference material' or 'reference standard' which has a true or assigned value for a constituent or property. One of the characteristics of a reference material or reference standard is that it must have a negligible sampling error between test portions.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1203

umpolung

Any process by which the normal alternating donor and acceptor reactivity pattern of a chain, which is due to the presence of O or N heteroatoms, is interchanged. Reactivity umpolung is most often achieved by temporary exchange of heteroatoms (N, O) by others, such as P, S and Se. The original meaning of the term has been extended to the reversal of any commonly accepted reactivity pattern. For example, reaction of R–C≡CX (X = halide) as a synthon for 'R–C≡C$^+$ (i.e. electrophilic acetylene) is an umpolung of the normal more common acetylide, R–C≡C$^-$ (i.e. nucleophilic) reactivity.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1174

unactivated adsorption process

If the temperature coefficient of the rate of adsorption is very small, the adsorption process is said to be unactivated (i.e. to have a negligible activation energy). In this case the sticking coefficient at low coverages may be near unity particularly for smaller molecules.

Source:
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 79

uncertainty of measurement

Parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand (the quantity being measured).

Source:
VIM

uniaxial pressing

Application of pressure in one direction during ceramization to achieve a uniform densification and the production of a compact monolith.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1826

uniaxial sample

Sample characterized by a (unique) sample axis Z with all directions perpendicular to Z being equivalent. In other words, the sample properties are invariant to rotation around Z. Uniaxiality exists in many anisotropic samples and simplifies the interpretation of their spectra considerably.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 437

unified atomic mass unit

Non-SI unit of mass (equal to the atomic mass constant), defined as one twelfth of the mass of a carbon-12 atom in its ground state and used to express masses of atomic particles, $\mathrm{u} \approx 1.660\,5402(10) \times 10^{-27}\ \mathrm{kg}$.

Source:
Green Book, 2nd ed., p. 75
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 997

uniform corrosion

Corrosion is uniform if the time average of the corrosion current through a unit area of any macroscopic dimension is independent of the position on the surface.

Source:
PAC, 1989, *61*, 19 *(Electrochemical corrosion nomenclature (Recommendations 1988))* on page 21

uniform polymer

A polymer composed of molecules uniform with respect to relative molecular mass and constitution.
Notes:

1. A polymer comprising a mixture of linear and branched chains, all of uniform relative molecular mass, is not uniform.
2. A copolymer comprising linear molecules of uniform relative molecular mass and uniform elemental composition but different sequential arrangements of the various types of monomeric units, is not uniform (e.g. a copolymer comprising molecules with a random arrangement as well as a block arrangement of monomeric units).
3. A polymer uniform with respect only to either relative molecular mass or constitution may be termed 'uniform', provided a suitable qualifier is used (e.g. 'a polymer uniform with respect to relative molecular mass').
4. The adjectives 'monodisperse' and 'polydisperse' are deeply rooted in the literature, despite the former being non-descriptive and self-contradictory. They are in common usage and it is recognized that they will continue to be used for some time; nevertheless, more satisfactory terms are clearly desirable. After an extensive search for possible replacements, the terms 'uniform' and 'non-uniform' have been selected and they are now the preferred adjectives.

Source:
PAC, 1996, *68*, 2287 *(Glossary of basic terms in polymer science (IUPAC Recommendations 1996))* on page 2301

uniformly labelled

A selectively labelled compound where all atoms of a particular element are labelled in the same isotopic ratio.

Source:
PAC, 1981, *53*, 1887 *(Nomenclature of inorganic chemistry: II.1 - Isotopically modified compounds)* on page 1895

uniformly labelled tracer

A tracer in which the label is uniformly distributed over its possible positions.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

unit cell

The smallest, regularly repeating material portion contained in a parallelepiped from which a crystal is formed by parallel displacements in three dimensions.

Notes:

1. Unlike in the case of low molar mass substances, the unit cell of polymer crystals usually comprises only parts of the polymer molecules and the regularity of the periodic repetition may be imperfect.
2. In the case of parallel-chain crystals, the chain axis is usually denoted by c or, sometimes, b.
3. This definition applies to the so-called primitive unit cell. In practice, the effective unit cell may consist of more than one primitive unit cell.

Source:
Purple Book, p. 76

unit (item/portion/individual)

in analytical chemistry

Each of the discrete, identifiable portions of material suitable for removal from a population as a sample or as a portion of a sample, and which can be individually considered, examined or tested, or combined. In the case of sampling bulk materials (or large packages), the units are increments, created by a sampling device. In the case of packaged materials, the unit may vary with the level of commercial distribution. For example, an individual piece of candy is the sampling unit at the consumer level; a package of individual pieces is the sampling unit at the retail level; a carton of packages is the sampling unit at the wholesale level; a pallet of cartons is the shipping unit at the distribution centre level; and a truckload of pallets is the consignment unit at the manufacture level. Before packaging, the bin containing the individual pieces would be the bulk lot (or batch) for sampling.

Source:
PAC, 1990, *62*, 1193 *(Nomenclature for sampling in analytical chemistry (Recommendations 1990))* on page 1202

unit

of measurement

Particular quantity, defined and adopted by convention, with which other quanitities of the same kind are compared in order to express their magnitudes relative to that quantity. Units have conventionally assigned names and symbols.

Source:
VIM
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 997

unit system

Set of base units, together with derived units, defined in accordance with given rules, for a given system of quantities.

Source:
VIM

universal calibration

in chromatography

A calibration of a size-exclusion chromatography set-up based on the finding that the retention volume of a molecular or particulate species is a single-valued function of an appropriate size parameter of this molecule or particle, irrespective of its chemical nature and structure. The product of the intrinsic viscosity and molar mass, $[\eta]M$, has been widely used as the size parameter.

Source:
Purple Book, p. 69

universal detector

in chromatography

A detector which responds to every component in the column effluent except the mobile phase.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 849

unperturbed dimensions

in polymers

The dimensions of an actual polymer random coil in a θ state.

Source:
Purple Book, p. 48

unreactive

Failing to react with a specified chemical species under specified conditions. The term should not be used in place of stable, since a relatively more stable species may nevertheless be more reactive than some reference species towards a given reaction partner.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1175

unstable

The opposite of stable, i.e. the chemical species concerned has a higher molar Gibbs energy than some assumed standard. The term should not be used in place of reactive or transient, although more reactive or transient species are frequently also more unstable. (Very unstable chemical species tend to undergo exothermic unimolecular decompositions. Variations in the structure of the related chemical species of this kind generally affect the energy of the transition states for these decompositions less than they affect the stability of the decomposing chemical species. Low stability may therefore parallel a relatively high rate of unimolecular decomposition.)

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1175

unstable film

See: stable film, metastable film

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 614

unstable ion

in mass spectrometry

An ion which is sufficiently excited to dissociate within the ion source.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1550

upconversion

The process by which two photons with frequencies ν_2 and ν_3 combine in a non-linear medium to produce a higher energy photon with frequency ν_1 such that $\nu_1 = \nu_2 + \nu_3$

Notes:

1. Also known as a parametric upconversion or sum frequency generation. Upconversion is the reverse process of downconversion.
2. The efficiency of the conversion process depends on the parametric gain in the non-linear material. This in turn depends on the power of the incident radiation, the photon frequencies, their indices of refraction in the material, and the non-linear 'hyper-susceptibility' of the material.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 437

upfield

See: chemical shift

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1175

uphill transport

in membrane processes

Process in which diffusion of a component occurs from a less concentrated stream to a more concentrated permeable stream.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1486

upper critical solution temperature

Recommended acronym: UCST

Critical temperature above which a mixture is miscible.
Notes:
1. Above the UCST and below the LCST, if it exists, a single phase exists for all compositions.
2. The UCST depends upon the pressure and molar-mass distributions of the constituent polymer(s).
3. For a mixture containing or consisting of polymeric components, these may be different polymers or species of different molar mass of the same polymer.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1999

upper limit of measurement

in atmospheric trace component analysis

Highest value of the air quality characteristic which can be measured by an instrument; its variations, caused for example by instability, are expected to lie within specified limits. The difference between the lower detection limit and the upper limit of measurement constitutes the dynamic range of the instrument.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2201

upstream

in membrane processes

Side of a membrane into which penetrants enter from the feed stream.

Source:
PAC, 1996, *68*, 1479 *(Terminology for membranes and membrane processes (IUPAC Recommendations 1996))* on page 1485

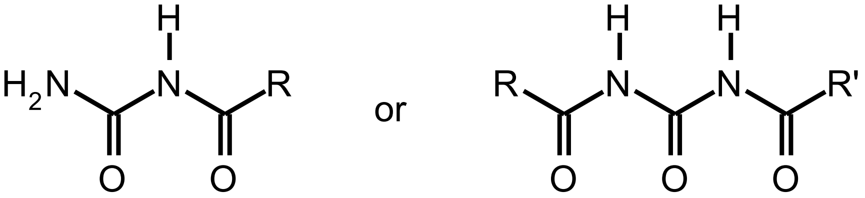
uptake

Entry of a substance into the body, into an organ, into a tissue, into a cell, or into the body fluids by passage through a membrane or by other means.

Source:
PAC, 2004, *76*, 1033 *(Glossary of terms used in toxicokinetics (IUPAC Recommendations 2003))* on page 1076

ureides

N-Acyl or *N,N'*-diacyl ureas.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

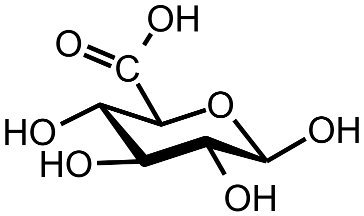
urethanes (urethans)

An alternative term for the compounds $R_2NC(=O)OR'$ ($R' \neq H$), esters of carbamic acids, $R_2NC(=O)OH$, in strict use limited to the ethyl esters, but widely used in the general sense, e.g. 'polyurethane resins'.
See: carbamates

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

uronic acids

Monocarboxylic acids formally derived by oxidation to a carboxy group of the terminal $-CH_2OH$ group of aldoses, e.g. D-glucuronic acid.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1373

See also:
White Book, p. 141

uronium salts

Salts of *O*-hydronated urea, having the structure $[HOC(=NH_2)NH_2]^+X^-$ (and *O*- and *N*- hydrocarbyl derivatives).

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

UV dose

A dose of ultraviolet (UV) radiation.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2283

UV photoelectron spectroscopy

Acronym: UPS

See: photoelectron spectroscopy

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2282
Orange Book, p. 250

UV stabilizer

A substance added to a sample to prevent photodeterioration by ultraviolet (UV) light.
See: photochemical reaction

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2283

vaccine

An agent containing antigens produced from killed, attenuated or live pathogenic microorganisms, synthetic peptides or by recombinant organisms, used for stimulating the immune system of the recipient to produce specific antibodies providing active immunity and/or passive immunity in the progeny.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 167

vacuum phototube

A photo-emissive detector inside an evacuated envelope with a transparent window, the photocathode, and the anode. The photocathode can be opaque or semitransparent.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1752

vacuum system

in mass spectrometry

Those components used to lower the pressure within a mass spectrometer are all parts of the vacuum system. This includes not only the various pumping components but also valves, gauges and associated electronic or other control devices, the chamber in which ions are formed and detected, and the vacuum envelope.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1546

valence

The maximum number of univalent atoms (originally hydrogen or chlorine atoms) that may combine with an atom of the element under consideration, or with a fragment, or for which an atom of this element can be substituted.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1175

valence band

Highest energy continuum of energy levels in a solid that is fully occupied by electrons at $0\ \mathrm{K}$.
Notes:

1. The valence band is lower in energy than the conduction band and is generally completely full in semiconductors. When heated, electrons from the valence band jump out of the band across the band gap and into the conduction band, making the material conductive. The Fermi level separates the valence band from the conduction band.
2. In metals the valence band is the conduction band.

3. Sample characterized by a (unique) sample axis Z with all directions perpendicular to Z being equivalent. In other words, the sample properties are invariant to rotation around Z. Uniaxiality exists in many anisotropic samples and simplifies the interpretation of their spectra considerably.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 438

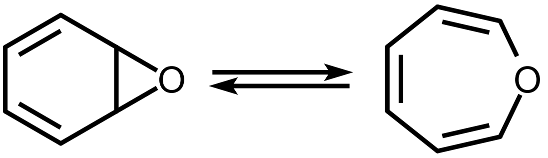
valence isomer

A constitutional isomer interrelated with another by pericyclic reactions. For example, Dewar benzene, prismane and benzvalene are valence isomers of benzene.
See: tautomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1175

valence tautomerization

The term describes simple reversible and generally rapid isomerizations or degenerate rearrangements involving the formation and rupture of single and/or double bonds, without migration of atoms or groups; e.g.



See also: fluxional, tautomerism

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1175

valence transition

A transition observed in certain rare-earth and actinide materials in which the electronic occupation of the 4f or 5f orbital changes with external conditions for example, temperature and pressure. Example: The transition at approximately 0.65 GPa where black, semiconducting $Sm^{2+}S^{2-}$ changes to golden metallic $(Sm^{3+}+e^{-})S^{2-}$.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 593

value of a division

of a precision balance scale

The reciprocal of the sensitivity; like the latter, it usually varies with load. It is determined by empirical calibration.

Source:
Orange Book, p. 35

value

of a quantity

Magnitude of a particular quantity generally expressed as a unit of measurement multiplied by a number.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 997

van der Waals adsorption

See: physisorption

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 586
PAC, 1976, *46*, 71 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units - Appendix II. Definitions, Terminology and Symbols in Colloid and Surface Chemistry. Part II: Heterogeneous Catalysis)* on page 75

van der Waals forces

The attractive or repulsive forces between molecular entities (or between groups within the same molecular entity) other than those due to bond formation or to the electrostatic interaction of ions or of ionic groups with one another or with neutral molecules. The term includes: dipole–dipole, dipole-induced dipole and London (instantaneous induced dipole-induced dipole) forces. The term is sometimes used loosely for the totality of nonspecific attractive or repulsive intermolecular forces.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1175

vaporization temperature, T_{vap}

in electrothermal atomization

The temperature of the atomization surface at which analyte loss becomes statistically significant.

Source:
PAC, 1992, *64*, 253 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - XII. Terms related to electrothermal atomization (IUPAC Recommendations 1992))* on page 257

vapour phase interference

in analysis

Interference caused by a change in the fraction of analyte dissociated, ionized or excited in the gaseous phase. (Note: here 'dissociation' means the formation of free neutral atoms from free molecules in the gaseous phase. The term atomization is here not appropriate because the latter also covers the formation of free atomic ions.) These interferences may be called dissociation, ionization and excitation interference, respectively.

Source:
Orange Book, p. 171

variable, x

The quantity or characteristic measured or computed. The corresponding numerical value may be taken for statistical handling; it may, for example, be a measured value or result.
Comment:
Note that statistical usage employs capital letters for random variables, and lower case for particular or observed values. In circumstances where the choice of 'x' as the symbol may cause confusion, another symbol may be used.
See also: dependent and independent variables

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 597

variable pathlength cell

in spectrochemical analysis

A cell whose pathlength can be varied either continuously or in steps by means of spacers.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1454

variance V, σ^2

The sum of the squares of the standard deviations, expressing the contributions to the overall precision from various sources of uncertainty.

Source:
Orange Book, p. 5

PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 601
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2218

variational transition state theory

This expression is applied to modifications of conventional transition state theory in which the position of the dividing surface in the potential-energy surface is varied. The rate is calculated with the surface at various positions, and the lowest rate calculated is taken to be closest to the truth.

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 190

Vavilov rule

See: Kasha–Vavilov rule

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2283

vector

in biotechnology

1. A DNA molecule (plasmid, virus, bacteriophage, artificial or cut DNA molecule) capable of being replicated and bearing cloning sites for the introduction of foreign DNA, used to introduce this DNA into host cells.
2. Any organism that transmits a disease between two hosts.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 168

velocity, v, c

Vector quantity equal to the derivative of the position vector with respect to time (symbols u, v, w for components of $\boldsymbol{c}$).

Source:
Green Book, 2nd ed., p. 11
ISO 31-1: 1992 *(Quantities and Units - Part 1: Space and Time.)*
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 997

velocity

in mass transport

The flux density $\boldsymbol{N}_{\mathbf{B}}$ is related to the velocity by the equation

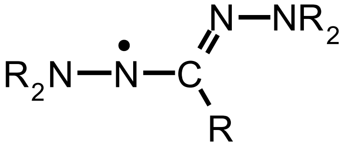
$$\boldsymbol{N}_{\mathbf{B}} = c_{\mathrm{B}}\, \boldsymbol{v}_{\mathbf{B}}$$

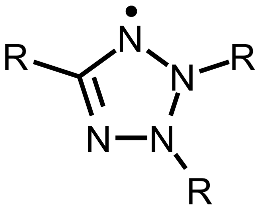
The vector $\boldsymbol{v}_{\mathbf{B}}$ is the macroscopic average velocity at which the species B moves (which is to be distinguished from the random molecular velocity); c_{B} is the concentration of species B ($\mathrm{mol\ m^{-3}}$). Note that the velocity is defined with respect to a frame of reference.

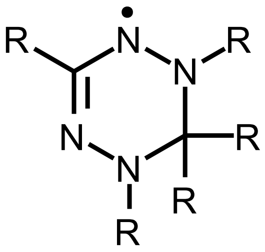
Source:
PAC, 1981, *53*, 1827 *(Nomenclature for transport phenomena in electrolytic systems)* on page 1830

verdazyl radicals

Relatively stable delocalized radicals, derived from hydrazyl, $H_2NN^{\cdot}H$, of the types shown, in particular the six-membered ring:







Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

vertical ionization

A process whereby an electron is removed from a molecule in its ground or an excited state so rapidly that a positive ion is produced without change in the positions or momenta of the atoms. The resultant ion is often in an excited state.

Source:
PAC, 1991, *63*, 1541 *(Recommendations for nomenclature and symbolism for mass spectroscopy (including an appendix of terms used in vacuum technology). (Recommendations 1991))* on page 1548

(vertical) rise velocity, v_f

in flame emission and absorption spectrometry

The vertical component of the velocity of the volatilized component in the observation space (in $\mathrm{mm\ s^{-1}}$). It depends on the flame temperature, the solute nebulized, the observation height and the gas flow rate.

Source:
PAC, 1986, *58*, 1737 *(Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))* on page 1742

Verwey transition

An electron-ordering transition occurring in a mixed-valent system that results in an ordering of formal valence states in the low-temperature phase. Example: The prototype system, first identified by Verwey, is the ferrospinel magnetite, $Fe^{3+}[Fe^{3+}Fe^{2+}]O_4$ in which an ordering of Fe^{3+} and Fe^{2+} ions within octahedral sites is thought to occur below $T_v \approx 120\ \mathrm{K}$.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 593

vibrational redistribution

Intramolecular redistribution of energy among the vibrational modes usually giving a statistical distribution of their populations, characterized by the 'vibrational temperature'. For large molecules, this process does not require collisions.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2283

vibrational relaxation

The loss of vibrational excitation energy by a molecular entity through energy transfer to the environment caused by collisions. The molecular entity relaxes into vibrational equilibrium with its environment.
See: relaxation

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2283

vibrational term, *G*

Vibrational energy divided by the product of the Planck constant and the speed of light.
See: term

Source:
Green Book, 2nd ed., p. 23

vibrationally adiabatic transition-state theory

See: adiabatic transition-state theory

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 190

vibronic coupling

Interaction between electronic and vibrational motions in a molecular entity.
See: Jahn–Teller effect, Renner–Teller effect

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2283

vibronic transition

A transition which involves a change in both the electronic and vibrational quantum numbers of a molecular entity, as opposed to purely electronic or purely vibrational transitions. The transition occurs between two states, just as in a purely electronic transition, but involves a change in both electronic and vibrational energy.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2283

vidicon

A vacuum tube containing a photosensitive area, or target, and an electron gun to read the signal from the target. The silicon target consists of a two-dimensional array of Si-photodiodes having a common cathode and isolated anodes. Irradiation of the target causes the production of electron-hole pairs which, by recombination, leads to a depletion of the surface charge.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1757

vinyl carbenes

Carbenes having a vinylic group on a carbenic carbon atom $R_2C{=}CRC{:}R \longleftrightarrow R_2C^+{-}CR{=}C^-R$. E.g. $H_2C{=}CHC{:}H$ prop-2-en-1-ylidene.
See: 1,3-dipolar compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

vinylic cations

Carbocations having the structure $R_2C{=}C^+{-}R$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

vinylic groups

The vinyl group ($CH_2{=}CH{-}$) and derivatives formed by substitution. Informally, a group, such as –OH, attached to the free valence of a (substituted) vinyl group is sometimes referred to as 'vinylic'.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

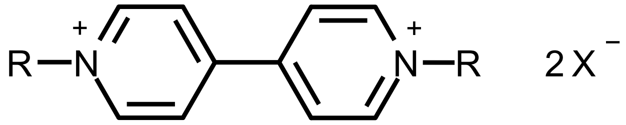
vinylidenes

Carbenes in which the carbenic carbon atom has a double bond to another carbon atom $R_2C{=}C{:}$, e.g. $H_2C{=}C{:}$ ethenylidene.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

viologens

1,1-Di(hydrocarbyl)-4,4'-bipyridinium salts.



Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

virial coefficients

Coefficients $(B, C, ...)$ in the virial equation of state for a real gas $p\, V_{\mathrm{m}} = R\, T \left(1 + \frac{B}{V_{\mathrm{m}}} + \frac{C}{{V_{\mathrm{m}}}^2} + ...\right)$ where p is the pressure, V_{m} the molar volume, R the gas constant and T the thermodynamic temperature.

Source:
Green Book, 2nd ed., p. 49

See also:
Purple Book, p. 58

virtual transition

A non-observable liquid-crystal transition that occurs below the crystallization temperature and is determined by extrapolation in binary phase diagrams.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 593

viscosity

See: dynamic viscosity

Source:
Green Book, 2nd ed., p. 13
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 997

viscosity function, $\varPhi$

A coefficient connecting the intrinsic viscosity, the radius of gyration and the molar mass of a chain macromolecule, according to the equation:

$$[\eta] = \frac{\varPhi\, 6^{\frac{3}{2}} \left(< s^2 > \right)^{\frac{3}{2}}}{M}$$

where $[\eta]$ is the intrinsic viscosity, s is the radius of gyration and M is the molar mass. The viscosity function is often referred to as the Flory constant.

Source:
Purple Book, p. 64

viscous sintering

Also contains definition of: viscous flow sintering

Sintering process by which it is possible to densify gels to glasses and ceramics at elevated temperatures.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1826

visibility

in atmospheric chemistry

Defined as the greatest distance at which a black object of suitable dimensions can be seen and recognized against the horizon sky, or, in the case of night observations, could be seen and recognized if the general illumination were raised to the normal daylight level. The criterion of recognizing the object, not just seeing the object without recognition, is used. Transmissometers, telephotometers and sun photometers are devices used to measure the degree of transmission of light. Nephelometers (integrating) are used to measure visibility by way of the light scattering from aerosols in the air mass.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2218

visible

Region of the electromagnetic spectrum extending from about $400\ \mathrm{nm}$ to $760\ \mathrm{nm}$. This is the wavelength region to which the human eye is sensitive. There are no precise limits for the spectral range of visible radiation since they depend upon the amount of radiant power reaching the retina and on the responsivity of the observer.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 439

volatilization

The conversion of a solid or liquid to a gas or vapour by application of heat, by reducing pressure, by chemical reaction or by a combination of these processes.

Example: $\mathrm{W(s)} + \frac{3}{2}\mathrm{O_2\,(g)} \rightarrow \mathrm{WO_3\,(g)}$

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 593

volatilizer

Material added to a sample to increase its volatilization or that of some component of it. Volatilizers increase the fraction volatilized either by forming more volatile compounds or by increasing the total surface area of all analyte particles (e.g. by explosive disintegration or by dispersal of the analyte in a highly volatile matrix).

Source:
Orange Book, p. 159
Orange Book, p. 172

volt

SI derived unit of electric potential, $\mathrm{V = J\,C^{-1} = m^2\,kg\,s^{-3}\,A^{-1}}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 997

voltage

in electroanalysis

The use of this term is discouraged, and the term applied potential should be used instead, for non-periodic signals. However, it is retained here for sinusoidal and other periodic signals because no suitable substitute for it has been proposed.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1505

voltammetric constant

In linear-sweep voltammetry and related techniques, the empirical quantity defined by the equation

$$\frac{i_p}{A\sqrt{v}\;c_{\mathrm{B}}} \quad \left(=\frac{j_p}{\sqrt{v}\;c_{\mathrm{B}}}\right)$$

where i_p is the peak current, A is the area of the electrode-solution interface, v is the rate of change of applied potential, and c_{B} is the bulk concentration of the substance B whose reduction or oxidation is responsible for the peak in question.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1505

volume content, V_c / m_s

The volume of an (isolated) specified component (C) divided by the mass of the system (S), e.g. patient–blood volume content. Volume content should not be confused with specific volume (or massic volume), which is the volume of the system divided by the mass of the system.

Source:
PAC, 1979, *51*, 2451 *(Quantities and units in clinical chemistry)* on page 2474

volume flow rate, q_v

Volume of a component crossing a surface divided by the time.

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 997

volume fraction, ϕ

Volume of a constituent of a mixture divided by the sum of volumes of all constituents prior to mixing.
See: fractions

Source:
Green Book, 2nd ed., p. 41
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 998

volume of activation, $\Delta^{\ddagger}V$

A quantity derived from the pressure dependence of the rate constant of a reaction (mainly used for reactions in solution), defined by the equation:

$$\Delta^{\ddagger}V = -R\,T\left(\frac{\partial(\ln k)}{\partial p}\right)_T$$

providing that the rate constants of all reactions (except first-order reactions) are expressed in pressure-independent concentration units, such as mol dm^{-3} at a fixed temperature and pressure. The volume of activation is interpreted, according to transition state theory, as the difference between the partial molar volumes of the transition state (V) and the sums of the partial volumes of the reactants at the same temperature and pressure, i.e.

$$\Delta^{\ddagger}V = {}^{\ddagger}V - \sum(r\,V_{\mathrm{R}})$$

where r is the order in the reactant R and V_{R} its partial molar volume.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1175

See also:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 191
Green Book, 2nd ed., p. 56

volume of the stationary phase

in chromatography

The volume of the stationary liquid phase or of the active solid or of the gel in the column. The volume of any solid support is not included.

Source:
Orange Book, p. 100

volume strain, θ

Also contains definition of: bulk strain

The change of volume divided by the original volume.

Source:
Green Book, 2nd ed., p. 12

volume viscosity (or dilatational viscosity)

A quantity ζ which enters into equations at any point where the flow involves a change in volume, i.e. is dilatational. If the deformation is purely dilatational, the average of three normal stress components is:

$$\sigma = \frac{1}{3}\left(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}\right) = -p + \zeta\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right)$$

where p is the hydrostatic pressure at the point considered in the absence of motion.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1216

volumetric flowrate

in gas chromatography

The flowrate of the mobile phase ($\mathrm{cm^3\ min^{-1}}$), normally specified at the column temperature and outlet pressure, although the measurement may be made at ambient temperature and must be corrected accordingly (and possibly also for water vapour present in the flowmeter).

Source:
Orange Book, p. 102

volumic

Attribute to a physical quantity obtained by division by volume. Charge density may thus be called volumic charge which is the electric charge in a section of space divided by the volume of that section.

Source:
ISO 31-0: 1992 *(Quantities and Units - Part 0: General Principles, Units and Symbols.)*
PAC, 1985, *57*, 1299 *(Review of plasma deposition applications: preparation of optical waveguides)* on page 1310
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 999

vulcanization

Chemical crosslinking of high-molar-mass linear or branched polymers to give a polymer network.
Notes:

1. The polymer network formed often displays rubber-like elasticity. However, a high concentration of crosslinks can lead to rigid materials.
2. A classic example of vulcanization is the crosslinking of *cis*-polyisoprene through sulfide bridges in the thermal treatment of natural rubber with sulfur or a sulfur-containing compound.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1826

VUV

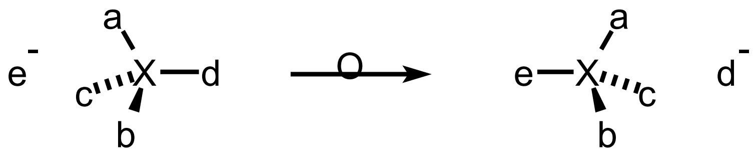
Acronym for vacuum ultraviolet.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 439

Walden inversion

Also contains definition of: retention of configuration

Retention of configuration is the preservation of integrity of the spatial arrangement of bonds to an chiral centre during a chemical reaction or transformation. It is also the configurational correlation when a chemical species Xabcd is converted into the chemical species Xabce having the same relative configuration. The configurational change when a chemical species Xabcd (where X is typically carbon), having a tetrahedral arrangement of bonds to X, is converted into the chemical species Xabce having the opposite relative configuration (or when it undergoes an identity reaction in which Xabcd of opposite configuration is produced) is called a Walden inversion or inversion of configuration. The occurrence of a Walden inversion during a chemical transformation is sometimes indicated in the chemical equation by the symbol shown below in place of a simple arrow pointing from reactants to products.



Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2221

wall-coated open-tubular (WCOT) column

in chromatography

A column in which the liquid stationary phase is coated on the essentially unmodified smooth inner wall of the tube.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 831

wash out

in atmospheric chemistry

The removal from the atmosphere of gases and sometimes particles by their solution in or attachment to raindrops as they fall.
See also: rain out *in atmospheric chemistry*

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2219

watt

SI derived unit of power, $W = J\ s^{-1} = m^2\ kg\ s^{-3}$.

Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 998

wave height (electrochemical)

The limiting current of an individual wave, frequently expressed in arbitrary units for convenience.

Source:
PAC, 1985, *57*, 1491 *(Recommended terms, symbols, and definitions for electroanalytical chemistry (Recommendations 1985))* on page 1505

wavefunction, Ψ, ψ, φ

Also contains definition of: state function

The solution of the Schrödinger equation, eigenfunction of the hamiltonian operator. Complex conjugate functions are denoted by an asterisk read as 'star'.

Source:
Green Book, 2nd ed., p. 16

wavelength, λ

Distance in the direction of propagation of a periodic wave between two successive points where at a given time the phase is the same.

Source:
Green Book, 2nd ed., p. 30
ISO 31-5: 1992 *(Quantities and Units - Part 5: Electricity and Magnetism.)*
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 998

See also:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2283
PAC, 1985, *57*, 105 *(Names, symbols, definitions and units of quantities in optical spectroscopy (Recommendations 1984))* on page 109

wavelength converter

A wavelength converter converts radiation at one wavelength to radiation at another detectable wavelength or at a wavelength of improved responsivity of the detector. The classical wavelength converter consists of a screen of luminescent material that absorbs radiation and radiates at a longer wavelength. Such materials are often used to convert ultraviolet to visible radiation for detection by conventional phototubes. In X-ray spectroscopy a converter that emits optical radiation is called a scintillator. In most cases wavelength conversion is from short to long wavelength, but in the case of conversion of long to short wavelength the process is sometimes called upconversion. Wavelengths of coherent sources can be converted using nonlinear optical techniques. A typical example is frequency doubling.

Source:
PAC, 1995, *67*, 1745 *(Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))* on page 1758

wavelength dispersion

in X-ray emission spectroscopy

Spatial separation of characteristic X-rays according to their wavelengths.

Source:
PAC, 1980, *52*, 2541 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - IV X-ray emission spectroscopy)* on page 2547

wavelength error

in spectrochemical analysis

The error in absorbance which may occur if there is a difference between the (mean) wavelength of the radiation entering the sample cell and the indicated wavelength on the spectrometer scale.

Source:
PAC, 1988, *60*, 1449 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VII. Molecular absorption spectroscopy, ultraviolet and visible (UV/VIS) (Recommendations 1988))* on page 1456

wavelength-dispersive X-ray fluorescence analysis

A kind of X-ray fluorescence analysis involving the measurement of the wavelength spectrum of the emitted radiation e.g. by using a diffraction grating or crystal.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

wavenumber, σ, $\tilde{\nu}$

The reciprocal of the wavelength, λ, or the number of waves per unit length along the direction of propagation. The SI unit is $\mathrm{m^{-1}}$, but a commonly used unit is $\mathrm{cm^{-1}}$. Symbols $\tilde{\nu}$ in a vacuum, σ in a medium.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2283
PAC, 1985, *57*, 105 *(Names, symbols, definitions and units of quantities in optical spectroscopy (Recommendations 1984))* on page 109
Green Book, 2nd ed., p. 30

weak collision

A collision between two molecules in which the amount of energy transferred from one to the other is not large compared to $k_B T$ (k_B is the Boltzmann constant and T the absolute temperature).

See: strong collision

Source:
PAC, 1996, *68*, 149 *(A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996))* on page 191

weathering

Exposure of a polymeric material to a natural or simulated environment.

Source:
PAC, 1996, *68*, 2313 *(Definitions of terms relating to degradation, aging, and related chemical transformations of polymers (IUPAC Recommendations 1996))* on page 2321

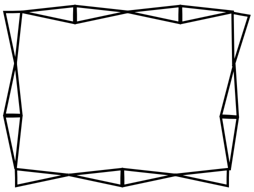
weber

SI derived unit of magnetic flux, $\mathrm{Wb} = \mathrm{V\ s} = \mathrm{m^2\ kg\ s^{-2}\ A^{-1}}$.

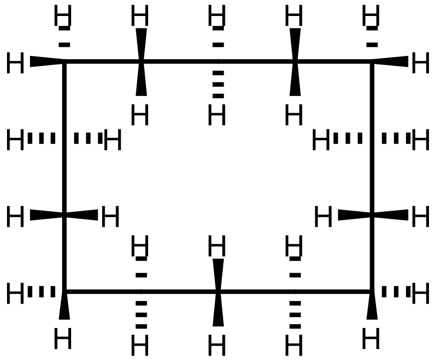
Source:
Green Book, 2nd ed., p. 72
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 998

wedge projection

A stereochemical projection, roughly in the mean plane of the molecule, in which bonds are represented by open wedges, tapering off from the nearer atom to the farther atom. It is mainly used to illustrate the conformation of larger cycloalkanes e.g. cyclotetradecane:



equivalent to



Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2222

weight, *G*

Force of gravity acting on a body, $G = m\,g$, where m is its mass and g the acceleration of free fall.

Source:
Green Book, 2nd ed., p. 12
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 999

weighted mean

If in a series of observations a statistical weight (w_i) is assigned to each value, a weighted mean $\bar{x}_w$ can be calculated by the formula:

$$\bar{x}_w = \frac{\sum w_i\,x_i}{\sum w_i}$$

Comment:
Unless the weights can be assigned objectively, the use of the weighted mean is not normally recommended.

Source:
PAC, 1994, *66*, 595 *(Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))* on page 599

Weller correlation

Empirical correlation for the energy of full charge-transfer exciplex relative to the ground state in *n*-hexane as a function of the electrochemical one electron standard reduction potential of the cation radical produced upon electron donation and standard reduction potential of the acceptor measured in a polar solvent for the donor (D) and the acceptor (A) involved

$$\Delta H(\mathrm{D^+A^-},\ \mathrm{hexane}) = e\,[E^0(\mathrm{D^{+\bullet}}/\mathrm{D}) - E^0(\mathrm{A}/\mathrm{A^{-\bullet}})] + e\,\Delta E$$

with $E^0(\mathrm{D^{+\bullet}}/\mathrm{D})$ and $E^0(\mathrm{A}/\mathrm{A^{-\bullet}})$ the standard electrode potentials of the donor and acceptor, respectively.
Notes:

1. In the case diethylaniline as donor and aromatic hydrocarbons as acceptors, the last term on the right, i.e., $e\,\Delta E = (0.15 \pm 0.10)$ eV. This equation assumes a constant Coulomb term and a constant entropy change within a particular series of partners. e is the elementary charge.
2. The IUPAC recommendations for the sign and symbols of standard potentials are used in the equation as written above.
3. Although not complying with the IUPAC recommended nomenclature for the standard electrode potentials, traditionally the equation has been written as:

   $$\Delta H(\mathrm{D^+A^-},\ \mathrm{hexane}) = e\,[E^0_{\mathrm{ox}} - E^0_{\mathrm{red}}] + (0.15 \pm 0.10)\ \mathrm{eV}$$

   with E^0_{ox} the standard electrode potential at which the oxidation occurs, and E^0_{red} the standard electrode potential at which the reduction occurs. This writing of the first term within the square brackets is misleading and not recommended.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 439

Westcott cross-section

See: effective thermal cross-section

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2517
Orange Book, p. 218

wet bulb temperature

In psychrometry, the temperature of the sensor or the bulb of a thermometer in which a constantly renewed film of water is evaporating. The temperature of the water used to renew the film must be at the temperature of the gas.

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2219

wetting

Process by which an interface between a solid and a gas is replaced by an interface between the same solid and a liquid.

Source:
PAC, 2004, *76*, 1985 *(Definition of terms related to polymer blends, composites, and multiphase polymeric materials (IUPAC Recommendations 2004))* on page 1991

wetting tension (or work of immersional wetting per unit area)

The work done on a system when the process of immersional wetting involving unit area of phase β is carried out reversibly:

$$w_{\mathrm{W}}^{\alpha\beta\delta} = \gamma^{\beta\delta} - \gamma^{\alpha\beta}$$

where $\gamma^{\alpha\beta}$ and $\gamma^{\beta\delta}$ are the surface tensions between two bulk phases α, β and β, δ, respectively.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 598

Wheland intermediate

See: Meisenheimer adduct, σ-adduct, arenium ions

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1176
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

Wiegner effect

Synonymous with suspension effect (in an ion-selective electrode).

Source:
PAC, 1994, *66*, 2527 *(Recommendations for nomenclature of ionselective electrodes (IUPAC Recommendations 1994))* on page 2533

Wigner matrices

See: molecular orientation

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Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 440

Wilzbach labelling

Labelling of a substance by exposing it to tritium gas.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2521

wind rose

Also contains definition of: pollution rose

A diagram designed to show the distribution of wind direction experienced at a given location over a considerable period of time. Usually shown in polar coordinates (distance from the origin being proportional to the probability of the wind direction being at the given angle usually measured from the north). Similar diagrams are sometimes used to summarize the average concentrations of a given pollutant seen over a considerable period of time as a function of direction from a given site (sometimes called a pollution rose).

Source:
PAC, 1990, *62*, 2167 *(Glossary of atmospheric chemistry terms (Recommendations 1990))* on page 2219

wolfram lamp

Incandescent lamp that generates light by passing an electric current through a thin filament wire (usually of wolfram) until it is extremely hot. The lamps are often filled by a halogen gas such as iodine and bromine that allow filaments to work at higher temperatures and higher efficiencies.
See: quartz–iodine lamp

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 440

Wood horn

A mechanical device that acts by absorption as a perfect photon trap.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2284

Wood lamp

Term used to describe a low-pressure mercury arc possessing a fluorescing layer, which emits in the UV-A region (from 315 to $400\ \mathrm{nm}$).

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 440

Woodward–Hoffmann rules

See: orbital symmetry

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1176

work, w, W

Scalar product of force, $\boldsymbol{F}$, and position change, $\mathrm{d}\boldsymbol{r}$, $w = \int \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{r}$.

Source:
Green Book, 2nd ed., p. 48
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 999

work hardening

Opposite of work softening, in which shear results in a permanent increase of viscosity or consistency with time.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

work of adhesion

Also contains definition of: work of separation

The work of adhesion per unit area, $w_{\mathrm{A}}^{\alpha\beta\delta}$, is the work done on the system when two condensed phases α and β, forming an interface of unit area are separated reversibly to form unit areas of each of the αδ- and βδ- interfaces.

$$w_{\mathrm{A}}^{\alpha\beta\delta} = \gamma^{\alpha\delta} + \gamma^{\beta\delta} - \gamma^{\alpha\beta}$$

where $\gamma^{\alpha\beta}$, $\gamma^{\alpha\delta}$ and $\gamma^{\beta\delta}$ are the surface tensions between two bulk phases α, β; α, δ and β, δ respectively. The work of adhesion as defined above, and traditionally used, may be called the work of separation.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 597

work of cohesion per unit area

Of a single pure liquid or solid phase α, w_{C}^{α} is the work done on the system when a column α of unit area is split, reversibly, normal to the axis of the column to form two new surfaces each of unit area in contact with the equilibrium gas phase.

$$w_{\mathrm{C}}^{\alpha} = 2\,\gamma^{\alpha}$$

where γ^{α} is the surface tension between phase and its equilibrium vapour or a dilute gas phase.

Source:
PAC, 1972, *31*, 577 *(Manual of Symbols and Terminology for Physicochemical Quantities and Units, Appendix II: Definitions, Terminology and Symbols in Colloid and Surface Chemistry)* on page 597

work softening

Also contains definitions of: shear breakdown, thixotropy

The application of a finite shear to a system after a long rest may result in a decrease of the viscosity or the consistency. If the decrease persists when the shear is discontinued, this behaviour is called work softening (or shear breakdown), whereas if the original viscosity or consistency is recovered this behaviour is called thixotropy.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

working electrode

An electrode that serves as a transducer responding to the excitation signal and the concentration of the substance of interest in the solution being investigated, and that permits the flow of current sufficiently large to effect appreciable changes of bulk composition within the ordinary duration of a measurement.

Source:
Orange Book, p. 60

worm-like chain

Also contains definition of: Porod–Kratky chain *in polymers*

Synonym: continuously curved chain *in polymers*

in polymers

A hypothetical linear macromolecule consisting of an infinitely thin chain of continuous curvature; the direction of curvature at any point is random. The model describes the whole spectrum of chains with different degrees of chain stiffness from rigid rods to random coils, and is particularly useful for representing stiff chains. In the literature this chain is sometimes referred to as a Porod–Kratky chain. Synonymous with continuously curved chain.

Source:
Purple Book, p. 51

ξ- (xi-)

A symbol used to denote unknown configuration at a chiral centre.

Source:
PAC, 1984, *56*, 595 *(Nomenclature and symbolism for amino acids and peptides (Recommendations 1983))* on page 601

x unit

Non-SI unit of length: $X \approx 1.002 \times 10^{-13}$ m

Source:
Green Book, 2nd ed., p. 110

X-radiation

Radiation resulting from the interaction of high energy particles or photons with matter.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 737

X-ray escape peak

In a gamma or X-ray spectrum, the peak due to the photoelectric effect in the detector and escape, from the sensitive part of the detector, of the X-ray photon emitted as a result of the photoelectric effect.

Source:
PAC, 1982, *54*, 1533 *(Glossary of terms used in nuclear analytical chemistry (Provisional))* on page 1541

X-ray fluorescence

The emission of characteristic X-radiation by an atom as a result of the interaction of electromagnetic radiation with its orbital electrons.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

X-ray fluorescence analysis

A kind of analysis based on the measurement of the energies and intensities of characteristic X-radiation emitted by a test portion during irradiation with electromagnetic radiation.

Source:
PAC, 1994, *66*, 2513 *(Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))* on page 2526

X-ray intensity

Essentially all X-ray measurements are made by photon counting techniques but the results are seldom converted to radiant flux or irradiance or radiant exposure. The term photon flux would be appropriate if the measurements were corrected for detector efficiency but this is seldom done for X-ray chemical analysis. Therefore the term X-ray intensity, I, is commonly used and expressed as photons/unit time detected. Likewise the term relative X-ray intensity, I_r, is used to mean the intensity for the analyte in an unknown specimen divided by the intensity for a known concentration of the analyte element.

Source:
PAC, 1980, *52*, 2541 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - IV X-ray emission spectroscopy)* on page 2544

X-ray level

An electronic state occuring as the initial or final state of a process involving the absorption or emission of X-ray radiation. It represents a many-electron state which, in the purely atomic case, has total angular momentum ($J = L + S$) as a well defined quantum number.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 737

X-ray photoelectron spectroscopy (XPS)

Any technique in which the sample is bombarded with X-rays and photoelectrons produced by the sample are detected as a function of energy. ESCA (Electron Spectroscopy for Chemical Analysis) refers to the use of this technique to identify elements, their concentrations, and their chemical state within the sample.

Source:
Orange Book, p. 250

X-ray satellite

Also contains definitions of: hypersatellite *in X-ray spectroscopy*, multiple ionization satellite *in X-ray spectroscopy* , non-diagram line *in X-ray spectroscopy*

A weak line in the same energy region as a normal X-ray line. Another name used for weak features is non-diagram line. Recommendations as to the use of these two terms have conflicted. Using the term diagram line as defined here, non-diagram line may well be used for all lines with a different origin. The majority of these lines originate form the dipole-allowed de-excitation of multiply ionized or excited states, and are called multiple-ionization satellites. A line where the initial state has two vacencies in the same shell, notably the K-shell, is called a hypersatellite. Other mechanisms leading to weak spectral features in X-ray emission are, e.g. resonance emission, the radiative Auger effect, magnetic dipole and electric quadrupole transitions and, in metals, plasmon excitation. Atoms with open electron shells, i.e. transition metals, lanthanides and actinides, show a splitting of certain X-ray lines due to the electron interaction involving this open shell. Structures originating in all these ways as well as structures in the valence band of molecules and solid chemical compounds have in the past been given satellite designations.

Source:
PAC, 1991, *63*, 735 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - VIII. Nomenclature system for X-ray spectroscopy (Recommendations 1991))* on page 739

X-ray spectroscopy

X-ray spectroscopy consists of three steps: (a) excitation to produce emission lines characteristic of the elements in the material, (b) measurement of their intensity, and (c) conversion of X-ray intensity to concentration by a calibration procedure which may include correction for matrix effects.

Source:
PAC, 1980, *52*, 2541 *(Nomenclature, symbols, units and their usage in spectrochemical analysis - IV X-ray emission spectroscopy)* on page 2544

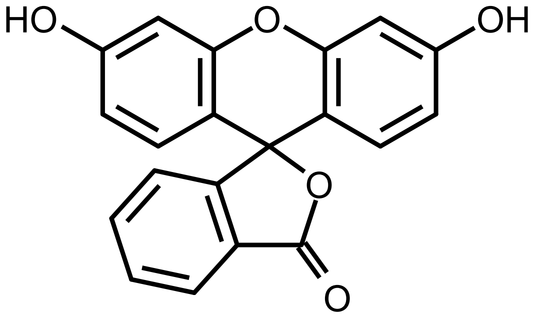
xanthates

See: xanthic acids

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

xanthene dyes

Dyes derived by condensation of phthalic anhydride with resorcinol (and derivatives) or *m*-aminophenol (and derivatives), of which fluorescein is the prototype (all such dyes have the xanthene nucleus).



See also: phthaleins, rhodamine dyes

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

xanthic acids [obsolete]

Compounds having the structure ROC(=S)SH. Thus *O*-esters of dithiocarbonic acid. Salts and esters of xanthic acid are xanthates. Use of this term is not recommended.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

xanthophylls

A subclass of carotenoids consisting of the oxygenated carotenes.

Source:
White Book, p. 226
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1374

xenobiotic

A xenobiotic (Greek, xenos 'foreign'; bios 'life') is a compound that is foreign to a living organism. Principal xenobiotics include: drugs; carcinogens; and various compounds that have been introduced into the environment by artificial means.

Source:
PAC, 1997, *69*, 1251 *(Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997))* on page 1303
This definition supersedes an earlier definition of xenobiotics.

xenon lamp

An intense source of ultraviolet, visible and near-infrared light produced by electrical discharge in xenon under high pressure.
See also: antimony–xenon lamp (arc), lamp, mercury–xenon lamp (arc)

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2284

xerogel

Open network formed by the removal of all swelling agents from a gel.
Notes:

1. Examples of xerogels include silica gel and dried out, compact, macromolecular structures, such as gelatin or rubber.
2. The definition proposed here is recommended as being more explicit.

Source:
PAC, 2007, *79*, 1801 *(Definitions of terms relating to the structure and processing of sols, gels, networks, and inorganic-organic hybrid materials (IUPAC Recommendations 2007))* on page 1808

Yang photocyclization

Intramolecular coupling of diradicals of different sizes (1,4-, 1,5-, 1,6-, 1,7-, 1,8-diradicals, as well as very remote diradicals) formed through intramolecular hydrogen abstraction by an excited ketone, yielding cyclic alcohols of different sizes.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 441

yard

Non-SI unit of length, $\mathrm{yd} = 3\ \mathrm{ft} = 0.9144\ \mathrm{m}$.

Source:
Green Book, 2nd ed., p. 110

year

Non-SI unit of time, $\mathrm{a} = 31\ 556\ 952\ \mathrm{s}$. The year is not commensurable with the day and not a constant. The value given corresponds to the Gregorian calendar year ($\mathrm{a} = 365.2425\ \mathrm{d}$).

Source:
Green Book, 2nd ed., p. 111

yield, Y

in biotechnology

Ratio expressing the efficiency of a mass conversion process. The yield coefficient is defined as the amount of *cell* mass (kg) or product formed (kg, mol) related to the consumed substrate (carbon or nitrogen source or oxygen in kg or moles) or to the intracellular ATP production (moles).

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 168

yield stress

The shear stress σ_0 or τ_0 at which yielding starts abruptly. Its value depends on the criterion used to determine when yielding occurs.

Source:
PAC, 1979, *51*, 1213 *(Manual of symbols and terminology for physicochemical quantities and units. Appendix II: Definitions, terminology and symbols in colloid and surface chemistry. Part 1.13. Selected definitions, terminology and symbols for rheological properties)* on page 1217

ylides

Also contains definition of: nitrogen ylides

Compounds in which an anionic site Y^- (originally on carbon, but now including other atoms) is attached directly to a heteroatom X^+ (usually nitrogen, phosphorus or sulfur) carrying a formal positive charge. They are thus 1,2-dipolar species of the type $R_mX^+–Y^-R_n$. If X is a saturated atom of an element from the first row of the periodic system, the ylide is commonly represented by a charge-separated form; if X is a second, third, etc. row element uncharged canonical forms are available $R_mX=YR_n$. If X is an unsaturated atom, doubly bonded to another first row element Z, the negative charge on Y may be stabilized by π-conjugation, $Z=X^+–Y^-R_n \longleftrightarrow Z^-–X^+=YR_n$. Such ylides belong to the class 1,3 dipolar compounds. However, 1,3-dipolar compounds with only sextet-containing canonical forms (e.g. vinylcarbenes) are not ylides. E.g. $Ph_3P^+–C^-H_2 \longleftrightarrow Ph_3P^+=CH_2$ (often called a Wittig reagent), $(CH_3)_3N^+–C^-H_2$, $RC\equiv N^+N^-–R$, $(CH_3)_2S=CHPh \longleftrightarrow (CH_3)_2S^+–C^-HPh$. Note that ylide is a complete word, not to be confused with the suffix -ylide, used for some radical anions. Subclasses of ylides: Ylides $R_mX^+–C^-R_2$ having the negative charge on carbon are classified by citing the name of the element X before the word ylide. E.g. nitrogen ylide, phosphorus ylide, oxygen ylide, *sulfur ylide*. A further specification may be achieved by citing the class name of R_mX before the word ylide. Thus nitrogen ylides include amine ylides, $R_3N^+–C^-R_2$, azomethine ylides $R_2C=N^+R–C^-R_2$, nitrile ylides, $RC\equiv N^+–C^-R_2$. Some authors, who wish to express the positive charge on X, prefer e.g. ammonium ylides over amine ylides; such usage varies according to the heteroatom X and to national custom. The ylides $R_mX^+–Y^- \longleftrightarrow R_mX=Y$ (Y = O, S, Se, Te, NR) are usually named by citing the name of R_mX followed by the additive nomenclature term for Y (oxide, sulfide, selenide, telluride, imide, respectively). E.g. amine imides; use of the less systematic synonyms amine imines

and aminimines is discouraged. Some classes of ylides are known by trivial names e.g. nitrones, Wittig reagents (synonymous with phosphonium ylides).
See also: betaines, dipolar compounds

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1375
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1176

ynamines

N,N-Disubstituted alk-1-yn-1-amines, $RC\equiv CNR_2$. By usage, restricted to this type of acetylenic amine.
See: enamines

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1375

ynols

Alk-1-yn-1-ols, $RC\equiv COH$; tautomeric with ketenes $RCH{=}C{=}O$.

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1375

yocto

SI prefix for 10^{-24} (symbol: y).

Source:
Green Book, 2nd ed., p. 74

yotta

SI prefix for 10^{24} (symbol: Y).

Source:
Green Book, 2nd ed., p. 74

Yukawa–Tsuno equation

A multiparameter extension of the Hammett equation to quantify the role of enhanced resonance effects on the reactivity of *meta*- and *para*-substituted benzene derivatives, e.g.

$$\log_{10}k = \log_{10}k_0 + \rho\,[\sigma + r\,(\sigma^{+} - \sigma)]$$

The parameter r gives the enhanced resonance effect on the scale $(\sigma^{+} - \sigma)$ or $(\sigma - \sigma)$, respectively.
See also: ρ-value, σ-constant

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1176

ζ-potential

See: electrokinetic potential

Source:
PAC, 1996, *68*, 957 *(Glossary of terms in quantities and units in Clinical Chemistry (IUPAC-IFCC Recommendations 1996))* on page 999

Z-value

An index of the ionizing power of a solvent based on the frequency of the longest wavelength electronic absorption maximum of 1-ethyl-4-methoxycarbonylpyridinium iodide in the solvent. The *Z*-value is defined by:

$$Z = \frac{2.859 \times 10^{4}}{\lambda}$$

where Z is in $\mathrm{kcal\ mol^{-1}}$ and λ is in nm.
See also: Dimroth–Reichardt E_{T} parameter, Grunwald–Winstein equation

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1176

Z_{50}

of a photochromic system

Number of cycles required to reduce by 50 % the initial absorbance of the coloured form of a photochromic compound at a specific wavelength.

Source:
PAC, 2007, *79*, 293 *(Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006))* on page 441

Zeeman effect

The splitting or shift of spectral lines due to the presence of an external magnetic field.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2284
Orange Book, p. 122

zepto

SI prefix for 10^{-21} (symbol: z).

Source:
Green Book, 2nd ed., p. 74

zero differential overlap (ZDO) approximation

An approach to the systematic neglect of the small-in-value electron repulsion integrals which is used in a number of approximate self-consistent field molecular orbital schemes. It means that all the products of atomic orbitals $\chi_\mu\ \chi_\nu$ are set to zero and the overlap integral $S_{\mu\nu} = \delta_{\mu\nu}$ (where $\delta_{\mu\nu}$ is the Kronecker delta). The ZDO approximation greatly simplifies the computation of wavefunctions by eliminating many of two-electron integrals. At the ZDO approximation all three- and four-centered integrals vanish.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1970

zero field splitting

The separation of multiplet sublevels in the absence of an external magnetic field.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2284

zero point

of a glass electrode

Value of the pH of a solution, which in combination with a stated outer reference electrode, gives zero emf from the operational cell.

Source:
PAC, 1985, *57*, 531 *(Definition of pH scales, standard reference values, measurement of pH and related terminology (Recommendations 1984))* on page 541

zero point of scale

of a balance

The rest point of the properly adjusted balance with no load on the pans and the rider (or chain) in the zero position.

Source:
Orange Book, p. 36

zero–zero (0–0) absorption or emission

A purely electronic transition occurring between the lowest vibrational levels of two electronic states.

Source:
PAC, 1996, *68*, 2223 *(Glossary of terms used in photochemistry (IUPAC Recommendations 1996))* on page 2284

zeta

See: ζ (beginning of `z`)

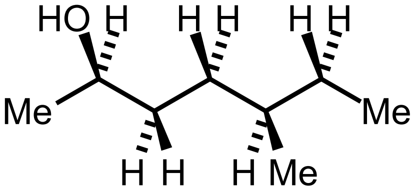
zetta

SI prefix for 10^{21} (symbol: Z).

Source:
Green Book, 2nd ed., p. 74

zig-zag projection

A stereochemical projection for an acyclic molecule (or portion of a molecule) where the main chain is represented by a zig-zag line in the plane and the substituents are shown above or below the plane.



Source:
PAC, 1996, *68*, 2193 *(Basic terminology of stereochemistry (IUPAC Recommendations 1996))* on page 2222

Zimm plot

A diagrammatic representation of data on scattering from large particles, corresponding to the equation:

$$\frac{K_c}{\Delta R(\theta)} = \frac{1}{\bar{M}_\mathrm{w}\, P(\theta)} + 2\, A_2\, c + \dots$$

and used for the simultaneous evaluation of the mass average molar mass, $\bar{M}_w$, the second virial coefficient of the chemical potential, A_2, and (usually) the z-average radius of gyration, $< s^2 >_z^{1/2}$; c is the mass concentration of the solute, $\Delta R(\theta)$ the excess Rayleigh ratio, and $P(\theta)$ the particle scattering function that comprises (usually) the z-average radius of gyration. K depends on the solute, the temperature and the type of radiation employed. Several modifications of the Zimm plot are in frequent use; the most common one uses the excess scattering instead of the excess Rayleigh ratio.

Source:
Purple Book, p. 66

zone

in chromatography

A region in the chromatographic bed where one or more components of the sample are located. The term band may also be used for it.

Source:
PAC, 1993, *65*, 819 *(Nomenclature for chromatography (IUPAC Recommendations 1993))* on page 824
Orange Book, p. 96

zone melting method of preconcentration

A technique based on the different solubility of microcomponents in the liquid and solid matrix. It has a limited field of application for the analysis of fusible (and stable) substances.

Source:
PAC, 1979, *51*, 1195 *(Separation and preconcentration of trace substances. I - Preconcentration for inorganic trace analysis)* on page 1200

Zucker–Hammett hypothesis

This hypothesis states that, if in an acid catalysed reaction, $\log_{10}k_1$ (first-order rate constant of the reaction) is linear in H_0 (Hammett acidity function), water is not involved in the transition state of the rate-controlling step. However, if $\log_{10}k_1$ is linear in $\log_{10}[H^+]$ then water is involved. This has been shown to be incorrect by Hammett himself.

Source:
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1176

zwitterionic compounds/zwitterions

Also contains definition of: dipolar ions

Synonym: inner salts

Neutral compounds having formal unit electrical charges of opposite sign. Some chemists restrict the term to compounds with the charges on non-adjacent atoms. Sometimes referred to as inner salts, dipolar ions (a misnomer). E.g. $H_3N^+CH_2C(=O)O^-$ ammonioacetate (glycine), $(CH_3)_3N^+–O^-$ trimethylamine oxide.
See: betaines, dipolar compounds, ylides

Source:
PAC, 1995, *67*, 1307 *(Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995))* on page 1375
PAC, 1994, *66*, 1077 *(Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994))* on page 1176

zwitterionic polymer

Synonym: polymeric inner salt

Ampholytic polymer containing ionic groups of opposite sign, commonly on the same pendant groups.

Source:
PAC, 2006, *78*, 2067 *(Terminology of polymers containing ionizable or ionic groups and of polymers containing ions (IUPAC Recommendations 2006))* on page 2074

zygote

The cell obtained as a result of complete or partial fusion of meiotically (cf. meiosis) produced cells.

Source:
PAC, 1992, *64*, 143 *(Glossary for chemists of terms used in biotechnology (IUPAC Recommendations 1992))* on page 168

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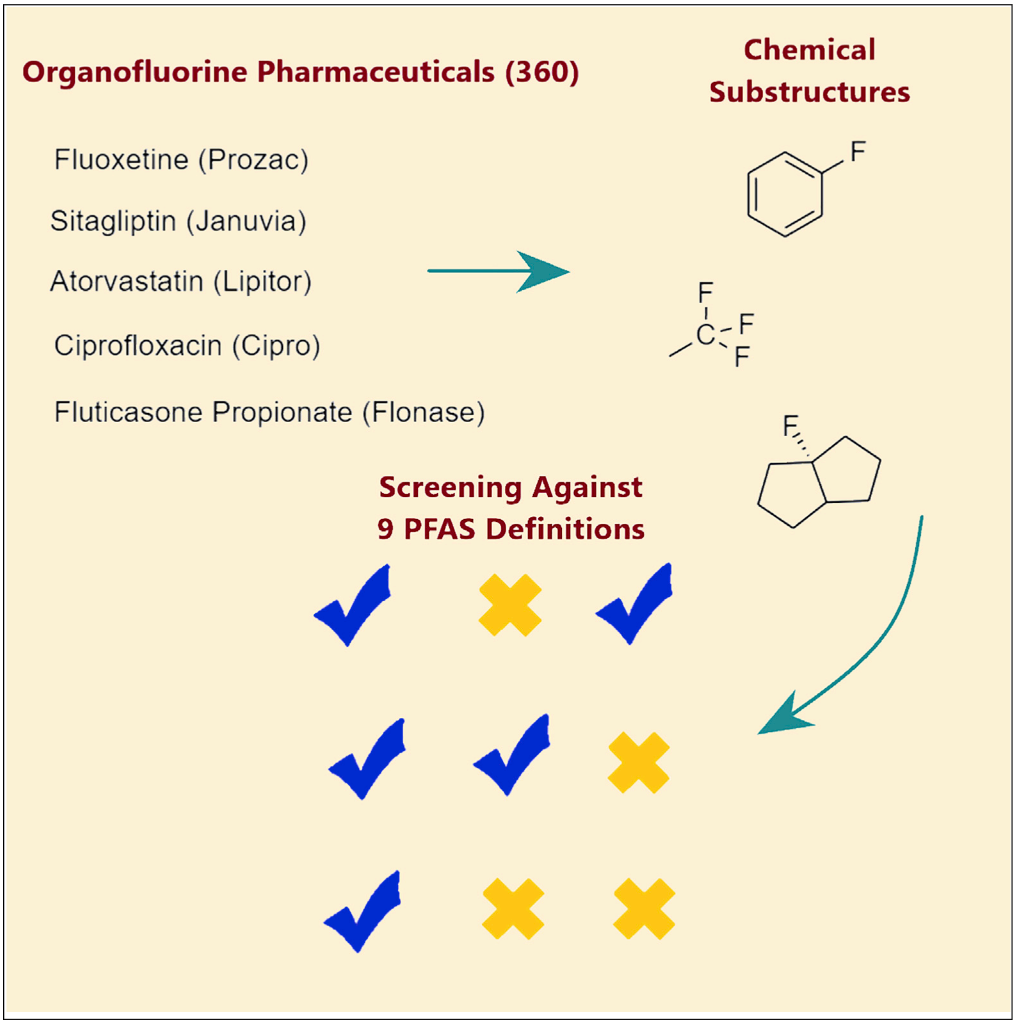
Implications of PFAS definitions using fluorinated pharmaceuticals



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Highlights

Nine PFAS definitions were evaluated and used to screen 360 organofluorine drugs

Broad definitions include many top prescribed pharmaceuticals, e.g., Prozac and Lipitor

Implications for fluorinated pharmaceuticals depend on intended use of the definition

Findings necessitate discussion of possible exemptions for pharmaceuticals

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Article

Implications of PFAS definitions using fluorinated pharmaceuticals

Emily Hammel,[1,3,*] Thomas F. Webster,[1] Rich Gurney,[2] and Wendy Heiger-Bernays[1]

SUMMARY

There are 9,000+ per- and polyfluoroalkyl substances (PFAS) in existence, which makes studying and regulating PFAS individually, or even as small mixtures, infeasible. Multiple PFAS definitions based on structure have been proposed, yet these definitions do not consider the implications for the full suite of organofluorine chemicals. For example, organofluorine pharmaceuticals, whose use may be essential and are found in human serum and wastewater, are not uniformly identified across all definitions. Using nine definitions prepared by various stakeholders, we screened the 360 organofluorine pharmaceuticals approved and used globally between 1954 and 2021. Definitions ranged in their inclusion of organofluorine pharmaceuticals (1%–100%). The most inclusive definitions include several top prescribed pharmaceuticals, e.g., Prozac and Lipitor. This analysis provides a framework against which organizations can make decisions about how best to proceed when defining PFAS.

INTRODUCTION

Since manufacturing began in the 1940s, per- and poly-fluoroalkyl substances (PFAS) have been widely used in textile manufacturing, food packaging, cookware, pesticide applicators, medical equipment, and other commercial products (Glüge et al., 2020). To date, upward of 9,000 PFAS have been identified (USEPA, 2021a). Many are toxic, persistent, and widely detected in the environment and human serum, prompting global discussion around their cost and benefits (Cordner et al., 2021), essential uses (Cousins et al., 2019), and effective strategies for regulation.

The large number of PFAS and the substitution of legacy compounds such as PFOA and PFOS by newer compounds—about which less is known although they may turn out to be just as problematic—has prompted movement away from the traditional chemical-by-chemical regulation toward regulation of these compounds as a class in both the U.S. (116th Congress, 2019; Kwiatkowski et al., 2020; Bălan et al., 2021) and Europe (ECHA, 2021). Several agencies, non-governmental organizations, and other groups have adopted class-based PFAS definitions for regulatory and non-regulatory purposes (Tables 1 and 2). Notably, the U.S. National Defense Authorization Act (NDAA) includes the PFAS Act of 2019, which adopts a structural definition classifying PFAS as any compound with at least ''one fully fluorinated carbon'' (116th Congress, 2019). The act authorizes funding for Department of Defense (DoD) initiatives related to PFAS remediation in areas impacted by military activities and sets restrictions on the use of PFAS in firefighting foam, personal protective equipment for firefighters, and food packaging used in military meals. Importantly, the act also sets requirements for environmental monitoring for PFAS in surface and groundwater and biomonitoring for PFAS among military personnel.

Recent work describes the advantages and disadvantages of different grouping strategies of PFAS based on their persistence and toxicity (Cousins et al., 2020; Wallington et al., 2021), yet relatively little work has been done to understand the differences between specific PFAS definitions and what set of compounds they will include. We focus here on organofluorine pharmaceuticals: they present an opportunity to assess the implications of PFAS definitions for a diverse but well-defined set of chemicals used globally. Organic fluorine was first introduced to the pharmaceutical industry in 1954 and is useful in altering the physiochemical properties of a drug to achieve a desired pharmacological effect (Inoue et tl., 2020). Pharmaceuticals represent a class of regulated chemicals whose use might be deemed at least partially ''essential'' for medical purposes. They are also of interest to environmental scientists for a number of reasons. For example, pharmaceutical waste enters the wastewater treatment systems (Kolpin et al., 2002), where metabolites are

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Table 1. Organizations, proposed and adopted definitions of PFAS, listed by year, evaluated in this analysis

Organization	Year	Regulatory?	Intended purpose
Buck et al.	2011	No	Establish clarity around the nomenclature of PFAS, including classifications based on molecular structure
OECD	2018, 2021	No	Characterize the universe of PFAS based on structural similarities between compounds containing fully fluorinated methyl or methylene moieties
Glüge et al.	2020	No	Understand major use areas; support work being done to address essentiality and feasibility of PFAS-free replacements
TURA Program, Massachusetts	2021a, 2021b	Yes	Establish new toxic substance category on toxic use inventory list in Massachusetts
U.S. EPA OPPT	2021	Yes	Lists chemicals for review under the Toxic Substances Control Act (TSCA) to evaluate risks to human health and the environment
NDAA, WA, CA, VT, ME[a] "≥1 Fully Fluorinated Carbon"	2019, 2020, 2021	Yes	Applications vary across agencies; reporting of PFAS in media impacted by military activities, ban of PFAS used in firefighting foam and equipment, and biomonitoring of PFAS in military personnel (NDAA); reporting and eventual ban of PFAS used in firefighting foam and firefighting equipment (CA); firefighting foam and food contact materials (WA); firefighting foam and products used in rugs/carpets/food packaging/ski wax (VT); any product containing intentionally added PFAS (ME).
NGOs[b] "All Organofluorine"	2021	No	Environmental advocacy; reflects organizations' broader mandates to protect constituents and the environment

[a] Authorities whose legislation defines PFAS as a class of fluorinated organic chemicals containing at least one fully fluorinated carbon atom.

[b] NGOs that advocate for broader definitions of PFAS to include all organofluorines.

either discharged back into the receiving waters, or are found in the biosolids after treatment (Massey and Waldron, 2011). While the degradation products of many pharmaceuticals remain unknown, active pharmaceutical ingredients and their metabolites are measurable in wastewater effluent (Yu et al., 2006). Models to predict biodegradability suggest some organofluorine pharmaceuticals may degrade into metabolites with trifluoromethyl groups and thus are likely to persist in the environment given the strength and durability of the CF_3-R functional group (Neuwoehner et al., 2009).

Definitions of PFAS are developed for multiple purposes, also referred to as "working scopes" (OECD, 2021), and can be both regulatory and non-regulatory. Regardless of its intended purpose, a useful definition requires clear, unambiguous language that is interpretable by stakeholders. In this analysis, we describe nine definitions of PFAS and examine some potential ambiguities in their language. We use each definition to screen a comprehensive list of organofluorine pharmaceuticals to determine which pharmaceuticals are included. Finally, we discuss some implications of these definitions given their intended purpose for use in regulatory or non-regulatory initiatives. Similar analyses could be performed for other groups of compounds.

RESULTS

Definitions of PFAS and their intended uses

Tables 1 and 2 show the nine PFAS definitions and their intended purpose. These include definitions developed by Buck et al. (2011), the Organisation for Economic Co-operation and Development (OECD), Glüge et al. (2020), the Toxic Use Reduction Act (TURA) Program of Massachusetts, U.S. EPA Office of Pollution Prevention and Toxics (U.S. EPA OPPT) (USEPA, 2021b), the NDAA (116th Congress, 2019) and laws from the states of Washington (2021), Vermont (2021), Maine (2021), and California (2020), and several non-governmental environmental advocacy organizations (e.g., Sierra Club of Massachusetts)

D11.4

Table 2. Definitions of PFAS included in analysis

Definition	Formal definition verbatim from organization	Informal interpretation
Buck et al. (2011)	"Aliphatic substances containing one or more C atoms on which all the H substituents present in the nonfluorinated analogues from which they are notionally derived have been replaced by F atoms, in such a manner that PFASs contain the perfluoroalkyl moiety C_nF_{2n+1}–."	Compounds that contain at least one carbon atom that is bound to three fluorine atoms (-CF_3). The structure must be saturated with no double or triple bonds (the only definition with this restriction).
OECD (2018)	"PFASs, including perfluorocarbons, that contain a perfluoroalkyl moiety with three or more carbons (i.e. –C_nF_{2n}–, $n \geq 3$) or a perfluoroalkylether moiety with two or more carbons (i.e. –$C_nF_{2n}OC_mF_{2m}$–, n and m $\geq$ 1)."	Compounds with at least three carbons on which all of the hydrogens have been replaced by a fluorine atom, so as to form a three-carbon unit with the subunits of (-CF_2-). It also includes compounds with an oxygen placed between two carbon atoms on which all of the hydrogens have been replaced by a fluorine atom, so as to form a carbon-oxygen-carbon unit with the subunits (-CF_2OCF_2-)
OECD (2021)	"PFASs are defined as fluorinated substances that contain at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it), i.e. with a few noted exceptions, any chemical with at least a perfluorinated methyl group (–CF_3) or a perfluorinated methylene group (–CF_2–) is a PFAS."	Compounds containing at least one carbon that has three fluorine atoms attached (–CF_3). Also includes compounds that have at least one carbon attached to two fluorine atoms (-CF_2-). In both cases, the carbon atom cannot be attached to a hydrogen, chlorine, or bromine atom. It still includes compounds whose carbon-fluorine units are attached together by an oxygen (-CF_2OCF_2-). These structures can contain rings or be arranged in a chain
Glüge et al. (2020)	In addition to substances containing C_nF_{2n+1}, where $n \geq 1$, it also "includes (i) substances where a perfluorocarbon chain is connected with functional groups on both ends, (ii) aromatic substances that have perfluoroalkyl moieties on the side chains, and (iii) fluorinated cycloaliphatic substances. Additionally, "polymeric PFAS with the –CF_2– moiety and non-polymeric PFAS with the –CF_2–CF_2– moiety … [excluding] non-polymeric substances that only contain a –CF_3 or –CF_2– moiety, with the exception of perfluoroalkylethers and per- and polyfluoroalkylether-based substances. For these two PFAS groups, substances with a –CF_2OCF_2– or –$CF_2OCFHCF_2$– moiety are also included."	Does not include compounds with a single –CF_2– or –CF_3, but can include compounds with two or more –CF_2– or –CF_3 groups. Compounds can contain rings or be arranged in a chain. Also includes compounds that contain two carbon atoms next to each other, each containing at least two fluorine atoms (–CF_2–CF_2–). The two fluorinated carbons can be attached together by an oxygen atom (–CF_2OCF_2– or –$CF_2OCFHCF_2$–).
TURA (2021a)	"Those PFAS that contain a perfluoroalkyl moiety with three or more carbons (e.g., –C_nF_{2n}–, $n \geq 3$; or CF_3–C_nF_{2n}–, $n \geq 2$) or a perfluoroalkylether moiety with two or more carbons (e.g., –$C_nF_{2n}OC_mF_{2m}$– or –$C_nF_{2n}OC_mF_m$–, n and m $\geq$ 1)."	Key to this definition is that the compound must contain a string of at least three carbon atoms, each containing two or more fluorine atoms. Perfluoroalkylethers are compounds that contain two –CF_2– groups connected by an oxygen. Includes linear, branched, cyclic compounds and aromatic rings
TURA (2021b)	"Certain PFAS not otherwise listed includes those PFAS that contain a perfluoroalkyl moiety with three or more carbons (e.g., –C_nF_{2n}–, $n \geq 3$; or CF_3–C_nF_{2n}–, $n \geq 2$) or a perfluoroalkylether moiety with two or more carbons (e.g., –$C_nF_{2n}OC_mF_{2m}$– or –$C_nF_{2n}OC_mF_m$, n and m $\geq$ 1), wherein for the example structures shown the dash (–) is not a bond to a hydrogen and may represent a straight or branched structure, that are not otherwise listed."	Clarifies that in TURA 2021a the (–) does not include a bond to hydrogen
U.S. EPA OPPT (2021)	"… a structure that contains the unit R-CF_2-CF(R′) (R″), where R, R′, and R″ do not equal "H" and the carbon-carbon bond is saturated (note: branching, heteroatoms, and cyclic structures are included)."	Compounds that contain a string of two adjacent carbon atoms, with one of them containing at least two fluorine atoms and the other containing at least one fluorine atom, and neither carbon bound to a hydrogen

(*Continued on next page*)

Table 2. *Continued*

Definition	Formal definition verbatim from organization	Informal interpretation
≥1 Fully Fluorinated Carbon[a]	Organic chemicals containing "at least one fully fluorinated carbon atom."	A compound with at least one carbon on which all of the hydrogen atoms have been replaced by fluorine atoms. The number of bonds on the carbon is not specified
All Organofluorine[b]	All organic compounds containing at least one fluorine atom should be classified as PFAS.	Any compound whose structure contains a carbon attached to a fluorine atom

[a] Authorities whose legislation defines PFAS as a class of fluorinated organic chemicals containing at least one fully fluorinated carbon atom (WA, VT, ME, CA, NDAA).

[b] NGOs that advocate for broader definitions of PFAS to include all organofluorines.

(Massachusetts Executive Office of Energy and Environmental Affairs, 2021). We consider two definitions proposed by the OECD, one from 2018 (OECD, 2018) and the update in 2021 (OECD, 2021). We also evaluated two definitions proposed by the TURA Program Administrative Council to the Massachusetts Department of Environmental Protection (MassDEP): the original definition developed by the TURA Science Advisory Board, represented as TURA (2021a) (Administrative Council on Toxics Use Reduction, 2021a), and an amended version clarifying the definition, represented by TURA 2021b (Administrative Council on Toxics Use Reduction, 2021b).

Screening organofluorine pharmaceuticals

Using the publicly available KEGG drug database (KEGG, 2021), 363 pharmaceuticals approved in the U.S., Japan, and Europe are identified including two over-the-counter drugs. Three compounds were excluded from analysis: the insecticide novaluron, the veterinary pharmaceutical dirlotapide, and sulfur hexafluoride (Lumason) which does not contain organically bound fluorine. The remaining 360 pharmaceuticals were included in the analysis: the complete list of chemical structures, therapeutic use areas, chemical identifiers, and numbers of prescriptions (where available) are provided in the supplemental information (Data S1).

Organofluorine pharmaceuticals can be organized by substructures within the compound. Figure 1 presents the frequency of substructures identified among the 360 fluorinated pharmaceuticals; 50% of organofluorine pharmaceuticals contain a single fluorine; 35% contain a single aromatic fluorine; 10% contain more than three fluorine atoms. Only four pharmaceuticals were fully or nearly fully fluorinated aliphatic compounds. There were 88 compounds containing at least one trifluoromethyl moiety (R-CF_3) where R is not hydrogen, 15 of which contained two trifluoromethyl moieties.

Table 3 summarizes the proportion of organofluorine pharmaceuticals that meet each of the nine structural definitions, disregarding for now their intended applications. The most inclusive is the "all-organofluorine" definition, including 100% of organofluorine pharmaceuticals. The revised TURA 2021b definition is least inclusive and captures the fewest (1.1%). We will now discuss each PFAS definition in roughly in the order in which they were proposed.

PFAS identified by Buck et al.

Buck et al. (2011) provided one of the earliest and most widely used of the PFAS definitions, replacing earlier terminology. According to Buck et al., PFAS are "aliphatic substances containing one or more C atoms on which all the H substituents present in the nonfluorinated analogs from which they are notionally derived have been replaced by F atoms, in such a manner that PFASs contain the perfluoroalkyl moiety C_nF_{2n+1}–." A restatement in less technical language is given in Table 2. Importantly, this definition excludes aromatic compounds (structures containing unsaturated hydrocarbon rings with double and single bonds). Based on this definition, 8 (2.2%) fluorinated pharmaceuticals would be classified as PFAS. An example of a fluorinated pharmaceutical compound meeting the definition outlined by Buck et al. is perflubron, a contrast imaging agent previously used in magnetic resonance imaging (MRI) scans which is now being investigated as liquid oxygen used to stabilize hemorrhage during major surgery (Figure 2A). While the Buck et al. definition is not regulatory, it has been adopted by the California Biomonitoring Program (OEHHA, 2021).

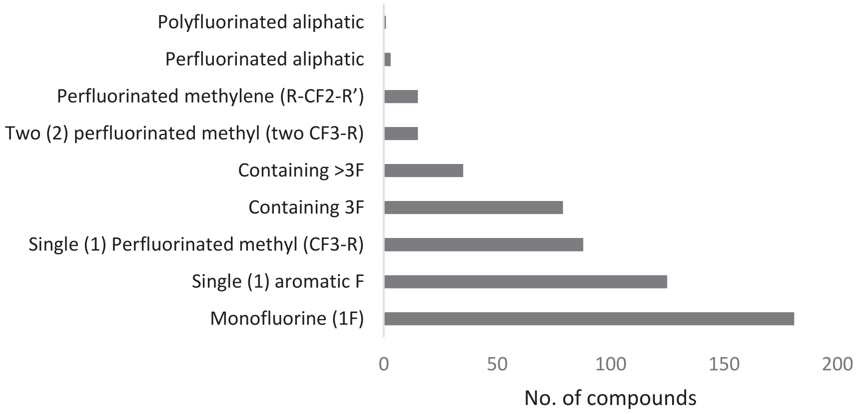


Figure 1. Substructures identified among organofluorine pharmaceuticals

PFAS identified by the Organisation for Economic Co-operation and Development (OECD)

The OECDoriginally defined PFAS as structures "that contain a perfluoroalkyl moiety with three or more carbons (i.e. $–C_nF_{2n}–$, $n \geq 3$) or a perfluoroalkylether moiety with two or more carbons (i.e. $–C_nF_{2n}OC_mF_{2m}–$, n and $m \geq 1$)" (OECD, 2018). Unlike Buck et al., this definition includes aromatic compounds. The OECD released a revised definition in 2021 including "fluorinated substances that contain at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it), i.e. with a few noted exceptions, any chemical with at least a perfluorinated methyl group ($–CF_3$) or a perfluorinated methylene group ($–CF_2–$)" (OECD, 2021). The revised definition reduced the number of carbons that must contain fluorine, but is clearer about the other atoms to which those carbons can be bonded. The 2018 OECD definition includes 5 (1.4%) organofluorine pharmaceuticals; the revised 2021 OECD definition includes 107 (30%) organofluorine pharmaceuticals. An example of a substance captured by the 2018 OECD definition but not Buck et al. is enflurane (Figure 2B). Included in the 2021 OECD definition but not Buck et al. are the cancer drug alpelisib (Figure 2C) and the widely used antidepressant fluoxetine (Prozac) (Figure 2G): the perfluorinated methyl groups warrant inclusion under the 2021 OECD definition, but the aromatic ring excludes them from Buck et al.

PFAS identified by Glüge et al.

The definition of Glüge et al. (2020) is broader than Buck et al., but narrower than the revised OECD 2021 definition (see Table 2 for the precise definition). Glüge et al. include aromatic compounds, similar to the OECD definition, yet does not include compounds with a single $–CF_3$ or $–CF_2–$, providing contrast to Buck et al. The antidiabetic medication gemigliptin meets the Glüge et al. definition because it is an aromatic substance that contains two perfluoroalkyl moieties on the side chains (Figure 2D). The Glüge et al. definition includes 22 (6.1%) organofluorine pharmaceuticals.

PFAS identified by the TURA Program of Massachusetts

The TURA Program originally defined PFAS as a compound containing "a perfluoroalkyl moiety with three or more carbons (e.g., $–C_nF_{2n}–$, $n \geq 3$; or $CF_3–C_nF_{2n}–$, $n \geq 2$) or a perfluoroalkylether moiety with two or more carbons (e.g., $–C_nF_{2n}OC_mF_{2m}–$ or $–C_nF_{2n}OC_mF_m–$, n and $m \geq 1$)" (Administrative Council on Toxics Use Reduction, 2021a). The slightly revised definition (Table 2) clarifies that the "–" excludes bonding to hydrogen. The original definition was ambiguous about this point and could be interpreted to include enflurane (Figure 2B) while the revised definition would not. Both would include perflexane (Figure 2E). The TURA 2021a definition includes six (1.7%) organofluorine pharmaceuticals while the revised definition includes four (1.1%).

PFAS identified by the U.S. EPA Office of Pollution Prevention and Toxics (OPPT)

The U.S. EPA OPPT defines PFAS as "… a structure that contains the unit $R\text{-}CF_2\text{-}CF(R')(R'')$, where R, R′, and R″ do not equal "H" and the carbon-carbon bond is saturated" (USEPA, 2021b). It also indicates that branched structures, heteroatoms, and cyclic structures are included. This definition is unambiguous, recognizing five (1.4%) organofluorine pharmaceuticals as PFAS. There were no compounds included

Table 3. Number of pharmaceuticals included under different definitions of PFAS (% of 360)

Definition	Number (%) organofluorine pharmaceuticals
Buck et al. (2011)	8 (2.2)
OECD (2018)	5 (1.4)
OECD (2021)	107 (30)
Glüge et al. (2020)	22 (6.1)
TURA (2021a)	6 (1.7)
TURA (2021b)	4 (1.1)
U.S. EPA OPPT (2021)	5 (1.4)
≥1 Fully Fluorinated Carbon[a]	337 (94)
All Organofluorine[b]	360 (100)

[a] Authorities whose legislation defines PFAS as a class of fluorinated organic chemicals containing at least one fully fluorinated carbon atom (NDAA, WA, ME, VT, CA).

[b] NGOs that advocate for broader definitions of PFAS to include all organofluorines.

under the OPPT definition that were not also captured by the 2021 OECDdefinition. Perflutren (Optison) is a contrast agent used in MRI and positron emission tomography (PET) imaging technology (Figure 2F). Perflutren meets all nine PFAS definitions examined as it is an aliphatic structure with three fully fluorinated carbon atoms (two perfluorinated methyl moieties and a perfluorinated methylene moiety).

PFAS identified by authorities as including at least one fully fluorinated carbon

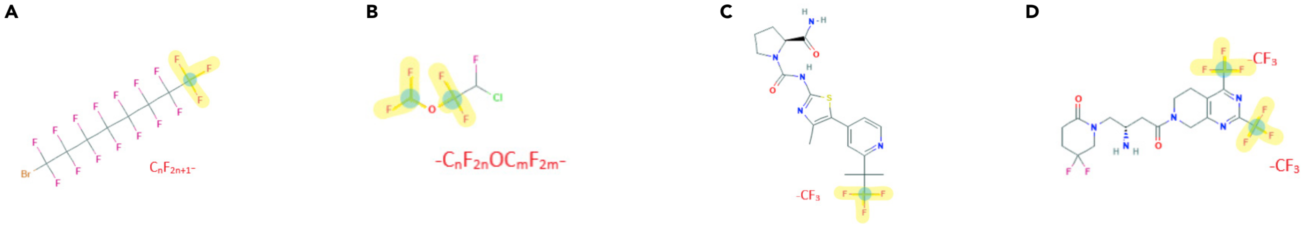
The U.S. NDAA defines PFAS as any substance containing "at least one fully fluorinated carbon" as do certain laws of the states of Washington, Vermont, Maine, and California (specific applications are discussed below). The NDAA defines a fully fluorinated carbon as "a carbon atom on which all of the hydrogen substituents have been replaced by fluorine" (116th Congress, 2019). However, the definition does not specify whether the fully fluorinated carbon is saturated or unsaturated (saturated compounds only contain single bonds). We therefore interpreted it to mean that the carbon could have single, double, or even triple bonds. This interpretation includes compounds containing a single fluorine atom attached to a benzene ring. As written, this definition captures 337 (94%) organofluorine pharmaceuticals. It includes the cholesterol-lowering medication atorvastatin (Lipitor), the top prescribed drug in the U.S. (Figure 2H) with 112,104,359 annual prescriptions (Table 4), as well as ciprofloxacin, a critical antibiotic (See Data S1). The ambiguity of the term "fully fluorinated carbon" is worth further consideration. If it had instead been interpreted to mean a trifluoromethyl group (R-CF_3) where R is not hydrogen, similar to Buck et al. (but without the latter definition's restriction to aliphatic compounds), neither Lipitor nor ciprofloxacin would be included, but Prozac (Figure 2G) would.

PFAS identified by non-governmental organizations: "all-organofluorine"

Some NGOs (Table 1) advocate for a broader definition of PFAS as any substance containing organofluorine. This definition is unambiguous and includes all 360 (100%) organofluorine pharmaceuticals, including widely used cancer chemotherapy drugs as well as Prozac and Lipitor discussed earlier.

DISCUSSION

The large number of PFAS listed by U.S. EPA and OECD suggests that research and regulation on a compound-by-compound basis is not practical. Multiple groups have devised definitions of PFAS to facilitate research into the prevalence, usage, and health effects of these substances, as well as serve as the basis for regulatory actions. Our analysis shows that the definitions have a very large range in the percent of organofluorine pharmaceuticals included. For this group of compounds, the definitions offer different and often conflicting views of what is and is not "PFAS". The framework we used is consistent with the systematic approach described in the OECD report (OECD, 2021) that provides practical guidance on characterizing PFAS based on molecular structure, and is similarly in line with the strategies described by (Wang et al., 2021) to facilitate unambiguous communication around PFAS. The cited examples serve to illustrate why PFAS definitions must be clear and that seemingly straightforward language—e.g., "fully fluorinated carbon"— can have multiple interpretations. Without specifying saturation (i.e., saturated compounds contain only single bonds), the fully fluorinated carbon definition can be interpreted to include any compound with

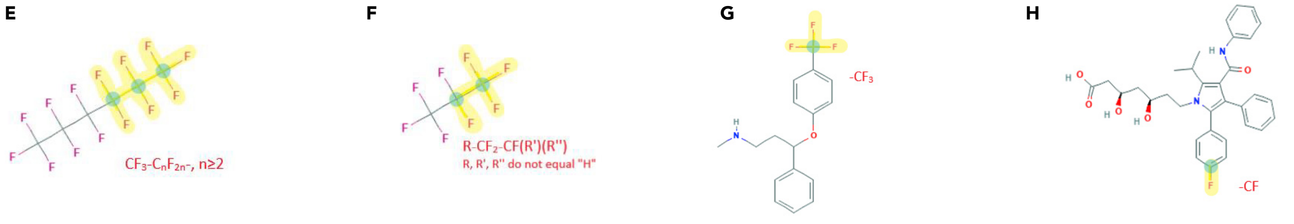


Perflubron
CAS No. 423-55-2

Enflurane
CAS No. 13838-16-9

Alpelisib
CAS No. 1217486-61-7

Gemigliptin
CAS No. 911637-19-9



Perflexane
CAS No. 355-42-0

Perflutren
CAS No. 76-19-7

Fluoxetine (Prozac)
CAS No. 54910-89-3

Atorvastatin (Lipitor)
CAS No. 134523-00-5

Figure 2. Examples of organofluorine pharmaceuticals that meet the nine PFAS definitions

(A) Buck et al. includes the contrast agent, perflubron (CAS No. 423-55-2).
(B) 2018 OECD and TURA 2021a both include the general anesthetic enflurane (CAS No. 13838-16-9).
(C) The 2021 OECD definition includes the antineoplastic alpelisib (CAS No.: 1217486-61-7).
(D) Glüge et al. includes the antidiabetic medication gemigliptin (CAS No. 911637-19-9).
(E) The TURA 2021b definition includes the cardiac ultrasound imaging agent perflexane (CAS No. 355-42-0).
(F) U.S. EPA OPPT includes the ultrasound contrast agent Perflutren (CAS No. 76-19-7).
(G) The ≥1 fully fluorinated carbon definition includes the antidepressant fluoxetine (Prozac) (CAS No. 54910-89-3).
(H) The "all-organofluorine" and ≥1 fully fluorinated carbon definitions include the cholesterol lowering medication atorvastatin (Lipitor) (CAS No. 134523-00-5).

a single aromatic fluorine, as well as other cases. While the definition was presumably intended to be clear and easy to interpret by stakeholders, it illustrates the importance of using specific and non-ambiguous language and being explicit in describing the context for which a definition shall be used.

To avoid confusion, it would ideally be useful to have a clear, universally agreed upon definition of PFAS. However, the appropriateness of a PFAS definition, or the possible need for exceptions in certain applications, may depend on the mandate of the group using the definition and its purpose. Of the nine definitions we have reviewed, five—Buck et al., OECD 2018 and 2021, Glüge et al., and "all organofluorines"—are non-regulatory at this time. The OECD, while not a regulatory institution, developed its own PFAS definition which may have regulatory implications if it is adopted by regulatory organizations, like the Registration, Evaluation, and Authorization of Chemicals (REACH) in the EU (European Commission, 2020). Five European countries (Germany, Netherlands, Denmark, Norway, and Sweden) announced their intention to develop a REACH restriction proposal for the European Commission that would cover all non-essential uses of PFAS in the EU (European Commission, 2020). Though not yet established at the time of this writing, this definition, if similar to the OECD, 2021 definition, may present important regulatory implications for the pharmaceutical industry and other producers of organofluorine chemicals.

Biomonitoring and environmental monitoring (e.g., of air and water) are critical surveillance aspects of environmental health. For example, biomonitoring of environmental chemicals is important for examining time trends (effectiveness of interventions, emerging problems, etc.) as well as geographical and demographic disparities and more. The definition used for PFAS has a potentially important role for biomonitoring, providing problem scoping, although there are practical limitations such as sample sizes, cost, availability of standards,

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Table 4. Classification of organofluorine pharmaceuticals that rank in the top 500 U.S. prescribed drugs from 2019 and global sales in USD

Drug name	Brand name	Therapeutic class	Total R_X (2019)[a]	Drug rank[b]	Global sales 2018 (millions)[c]	All-organofluorine	$\geq$1 Fully fluorinated carbon	OECD (2021)	TURA (2021a)	TURA (2021b)	Gluge et al	Buck et al	OECD (2018)	U.S. EPA OPPT
Flecainide	Tambocor	Tachyarrhythmia	2,318,516	215	296	X	X	X	X	X	X			
Fluoxetine	Prozac, Sarafem	antidepressant	27,110,302	20	945	X	X	X						
Celecoxib	Celebrex	NSAID; arthritis	6,595,235	102	3,980	X	X	X						
Levofloxacin	Iquix, Levaquin	Antibiotic	3,202,649	182	432	X	X	X						
Dexlansoprazole	Dexilant	proton pump inhibitor	2,290,526	218	3,831	X	X	X						
Leflunomide	Arava	rheumatoid arthritis	1,057,644	324	420	X	X	X						
Sulindac	Clinoril	NSAID	318,884	408	30	X	X	X						
Atorvastatin	Lipitor	cholesterol lowering agent	112,104,359	1	7,414	X	X							
Pantoprazole	Protonix	proton pump inhibitor	28,880,217	16	569	X	X							
Fluticasone propionate	Flonase	glucocorticoid (OTC)	27,893,102	18	791	X	X							
Escitalopram	Lexapro	antidepressant	27,510,958	19	1,282	X	X							
Rosuvastatin	Crestor	cholesterol lowering agent	27,041,319	21	n/a	X	X							
Citalopram	Celexa	antidepressant	21,546,700	30	n/a	X	X							
Sitagliptin	Januvia	antidiabetic	8,866,811	88	24,250	X	X							
Triamcinolone	Aristocort; Trianex	corticosteroid	6,320,751	107	n/a	X	X							
Ezetimibe	Zetia	cholesterol lowering agent	6,221,674	108	8,865	X	X							
Ciprofloxacin	Cipro	Antibiotic	5,878,441	113	488	X	X							
Fluconazole	Diflucan	antifungal	5,149,547	133	371	X	X							
Risperidone	Perseris Kit, Risperdal	antipsychotic	4,285,907	149	2,795	X	X							
Clobetasol	Clobex	corticosteroid	3,226,423	180	1,485	X	X							
Nebivolol	Bystolic	antihypertensive agent	3,061,887	191	2,800	X	X							
Ticagrelor	Brilinta	anticoagulant	2,299,436	216	3,007	X	X							
Ofloxacin	Floxin	antibiotic	2,051,823	232	153	X	X							

(*Continued on next page*)

Table 4. *Continued*

Drug name	Brand name	Therapeutic class	Total R_X (2019)[a]	Drug rank[b]	Global sales 2018 (millions)[c]	All-organofluorine	≥1 Fully fluorinated carbon	OECD (2021)	TURA (2021a)	TURA (2021b)	Gluge et al	Buck et al	OECD (2018)	U.S. EPA OPPT
Canagliflozin	Invokana	antidiabetic	1,373,540	290	4,327	X	X							
Betamethasone	Celestone, Alphatrex	corticosteroid	1,311,106	296	n/a	X	X							
Betamethasone dipropionate		corticosteroid	1,311,106	296	498	X	X							
Fluocinonide	Lidex	corticosteroid	1,290,749	300	555	X	X							
Travoprost	Izba, Travatan	glaucoma	1,264,924	303	2,722	X	X							
Difluprednate	Durezol	corticosteroid	717,461	356	587	X	X							
Dexamethasone	Decaderm, Decadron	corticosteroid	711,271	359	381	X	X							
Moxifloxacin	Avelox	antibiotic	666,288	363	n/a	X	X							
Fluorouracil	Adrucil, Carac, Efudex	antineoplastic	642,441	364	447	X	X							
Fluorometholone	Oxylone, Flarex	corticosteroid	434,531	389	161	X	X							
Fluocinolone acetonide	Flucinolone, Capex	corticosteroid	313,715	410	153	X	X							
Flurbiprofen	Ansaid	NSAID	21,338	477	6	X	X							
Emtricitabine	Emtriva	antiretroviral	3,632	501	5,457	X	X							
Paroxetine	Paxil	antidepressant	9,783,755	78	741	X								
Lansoprazole	Prevacid	propton pump inhibitor	2,772,218	200	963	X								
Diflunisal	Dolobid	NSAID	116,622	441	20	X								

[a] Annual prescription data for organofluorine pharmaceuticals are available from ClinCalc DrugStats database for the top 500 prescribed drugs in the U.S. for 2019.

[b] Drug Rank represents the rank order by frequency prescribed within a calendar year in the U.S.; data were compiled from the ClinCalc DrugStats database.

[c] Global sales data reported by PharmaCompass include prescriptions covered under Medicaid.

detection limits, etc. Biomonitoring programs may not be interested in organofluorine pharmaceuticals (e.g., the widely used Lipitor) themselves, except perhaps to try to close some of the gap between currently measured PFAS in serum vs. extractable organic fluorine (Yeung et al., 2008). Instead, biomonitoring programs would be more likely to examine the trends of known PFAS and add emerging compounds as they are discovered. California Biomonitoring currently uses the Buck et al. definition of PFAS (which would include very few organofluorine pharmaceuticals) (OEHHA, 2021). As discussed earlier, the PFAS definition included in the NDAA—which requires biomonitoring for PFAS among all military firefighters during their annual exam—uses the very broad and ambiguous ''fully fluorinated carbon'' definition, which includes over 90% of organofluorine drugs. Both of these applications may consider exempting such compounds.

On the other hand, monitoring of surface water, wastewater, biosolids, and other environmental media may be more interested in organofluorine pharmaceuticals as well as more traditional PFAS. Here, the definition of PFAS could well have regulatory implications and the choice of definition and possible exceptions would need to be carefully considered. For example, the NDAA applies the ''fully fluorinated carbon'' definition to environmental monitoring of PFAS in surface and groundwater by the United States Geological Survey (116th Congress, 2019). Recent efforts to measure total organic fluorine (TOF) in surface water (Ruyle et al., 2021) and in animal serum (Yeung et al., 2009) show that only a fraction of extractable organic fluorine (EOF) can be explained by known (targeted) PFAS, leaving a substantial portion of unidentified fluorine from other sources. Given the fate of organofluorine pharmaceuticals in wastewater, it is likely that these compounds would contribute to EOF measured in wastewater, and authorities that use the ''fully fluorinated carbon'' definition to measure or regulate PFAS will need to consider the implications for organofluorine pharmaceuticals. Alternatively, if the U.S. EPA OPPT definition were used, only a handful of organofluorine pharmaceuticals would be included. As a result, most pharmaceutical compounds, for which very little is understood on the biodegradability and recombination of breakdown products, would not be measured.

Four of the definitions we have considered—TURA 2021a/b, U.S. EPA OPPT, and the ''fully fluorinated carbon'' definition used by several states and the NDAA—have regulatory implications. There are important challenges around clarity and feasibility of regulating substances as a class. Ambiguities in how a definition is interpreted and applied can lead to misinterpretations by stakeholders, raising the likelihood of legal ramifications and ultimately slowing the process, potentially defeating the original goal of accelerating regulation through assessing PFAS on the basis of classes rather than individual chemicals. Earlier, we discussed the ambiguity in the ''fully fluorinated carbon'' definition and how it dramatically increased the number of organofluorine pharmaceuticals included. This would likely be true of other groups of organofluorine compounds not classified as PFAS under many of the other definitions.

Legislation in Washington, Vermont, California, and Maine (as well as the NDAA discussed above) each define PFAS as any compound containing at least one fully fluorinated carbon, but the applications differ. In California, the fully fluorinated carbon definition applies specifically to PFAS used in firefighting equipment and aqueous film forming foam (AFFF) (California, 2020). In Washington, this definition is applied to AFFF and food contact materials (Washington, 2021). Vermont applies the definition to AFFF as well as products added to rugs, food packaging, and ski wax (Vermont, 2021). When applied in these cases, the definition would not include organofluorine pharmaceuticals. Maine applies the fully fluorinated carbon definition in its legislation banning the selling or importing of any product containing intentionally added PFAS (Maine, 2021). The language of this legislation recognizes product categories in which the use of PFAS is currently unavoidable, which may include pharmaceuticals. Maine would also exempt pharmaceuticals because they are already regulated under federal law. Without this recognition, this law would include 94% of organofluorine pharmaceuticals.

The Massachusetts Toxic Use Reduction legislation provides an interesting example of exceptions. Certain industrial sectors are exempt from reporting toxic substances (MassDEP, 2018), including hospitals that may generate waste containing fluorinated contrast agents or other organofluorine pharmaceuticals used during hospital-based activities (e.g., surgical procedures, ventilation, etc.). Another approach to exceptions relevant to organofluorine pharmaceuticals is whether such products are deemed essential (Cousins et al., 2019).

Importantly, the list of organofluorine pharmaceuticals is dynamic and new drugs containing fluorine are developed each year. In fact, five organofluorine pharmaceuticals were approved during the final months of 2021, including Pfizer's new drug Paxlovid, the first protease inhibitor for treatment of SARS-CoV-2

(Pfizer, 2021). Pfizer signed a licensing agreement in November 2021 that will enable qualified manufacturers to produce and distribute the drug globally in order to reach a wider range of the global population (Pfizer, 2021). Paxlovid is an organofluorine pharmaceutical that meets the criteria of the revised OECD definition, the all-organofluorine definition, as well as the fully fluorinated carbon definition.

Moving forward with a useful framework

The definitions may be characterized by three attributes: clarity, inclusion, and specificity. Clarity may be interpreted as the degree to which a particular definition is open to conflicting decisions on whether a given PFAS structure meets the stated definition. Next, inclusion may be interpreted as the extent to which a definition would label any organofluorine compound as "PFAS", which we have illustrated here with pharmaceuticals. By specificity, we mean usefulness for its intended purpose. Specificity may be of particular importance to monitoring and regulatory bodies, which may need to consider exemptions for certain types of organofluorines if broad PFAS definitions are used. While consideration of these factors is important as we move forward, the real danger is not adopting any definition, for fear of not having a perfect definition, and the consequential delay in decision making.

Limitations of the study

This analysis considers nine available definitions of PFAS, yet new definitions may be developed for unique purposes, and previously established definitions may be revised in the future. Only those definitions available in the public space were included in this analysis. We include a comprehensive list of organofluorine pharmaceuticals approved between 1954 through June 1, 2021, including compounds that have been withdrawn. New therapeutics containing organofluorine approved after June 1, 2021 are not included. Our analysis is limited to human pharmaceuticals and does not include pharmaceuticals used in animals. Finally, available data on annual prescriptions are limited to the most widely prescribed drugs.

GLOSSARY

Aliphatic: saturated organic compounds in which the carbon atoms may form an open chain or closed rings

Alkyl group: a portion of a compound made up by carbon and hydrogen atoms arranged in a chain and whose structure follows the formula C_nH_{2n+1}

Aromatic: organic compounds containing a planar unsaturated ring of atoms that is stabilized by an interaction of the bonds forming the ring. Such compounds are typified by benzene and its derivatives

Ether: organic functional group typified by an oxygen atom connected to two carbon atoms, which may be aliphatic, olefinic, or aromatic.

Methyl group: a small molecule consisting of one carbon and three hydrogen atoms –CH3

Methylene group: a small molecule consisting of one carbon attached to two hydrogen atoms –CH2–

Moiety: a portion of a molecule with its own functional group

Olefinic: unsaturated organic compounds in which the carbon atoms may form an open chain or closed rings, including carbons that are double or triple bonded to another carbon.

Perfluorinated: a term to describe a hydrocarbon chain in which all of the hydrogen atoms are replaced by fluorine atoms

PFAS: per- and poly-fluoroalkyl substance

Polyfluorinated: a hydrocarbon chain in which multiple but not all hydrogen atoms are replaced by fluorine atoms

Polymer/polymeric: a class of compounds composed of macromolecules, usually consisting of multiple, repeating units called monomers

STAR★METHODS

Detailed methods are provided in the online version of this paper and include the following:

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SUPPLEMENTAL INFORMATION

Supplemental information can be found online at https://doi.org/10.1016/j.isci.2022.104020.

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AUTHOR CONTRIBUTIONS

Conceptualization, E.H., T.W., and W.H-B.; Methodology, E.H., T.W., R.G., and W.H-B.; Writing, E.H., T.W., W.H-B., and R.G.

DECLARATION OF INTERESTS

W.H-B and R.G. are members of the Toxic Use Reduction Institute Science Advisory Board in Massachusetts. The authors declare no other competing interests.

INCLUSION AND DIVERSITY

One or more of the authors of this paper self-identifies as a member of the LGBTQ+ community. One or more of the authors of this paper received support from a program designed to increase minority representation in science.

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STAR★METHODS

KEY RESOURCES TABLE

REAGENT or RESOURCE	SOURCE	IDENTIFIER
Other		
Chemical Structures and identifiers	National Library of Medicine PubChem Database	https://pubchem.ncbi.nlm.nih.gov/
Drug Database	KEGG Drug Databaste: Krypto Encyclopedia of Genes and Genomes	https://www.genome.jp/kegg/drug/
Prescription Drug Data	ClinCalc DrugStats Database	https://clincalc.com/
Global Sales Data	PharmaCompass Database	https://www.pharmacompass.com/

RESOURCE AVAILABILITY

Lead contact

Further information and requests for resources should be directed to and will be fulfilled by the lead contact, Emily Hammel (eghammel@bu.edu).

Materials availability

This study did not generate new materials.

Data and code availability

This paper analyzes existing, publicly available data. The data generated in this manuscript are supplied in a supplemental table. Any additional information required to reanalyze the data reported in this paper is available from the lead contact upon request. This paper does not report original code.

METHOD DETAILS

Identifying PFAS definitions

We selected and reviewed nine adopted definitions of PFAS that were available at the time of writing developed by both regulatory and non-regulatory organizations, presented in Table 1. Selection was based on the availability of a PFAS definition and a traceable description of the purpose for the development of the definition as it fits into the organizations' mandates or working scope. We present the organizations chronologically based on when the definition of PFAS was developed. For the purposes of direct comparison, we present the updated definitions for two of the organizations together with the originally developed definition.

Organofluorine pharmaceutical database

To establish a comprehensive list of organofluorine pharmaceuticals registered globally to date, we extended the work by Inoue et al. (2020), which included pharmaceuticals approved between 1954 and 2019, by querying the KEGG Drug database (Release version 99.1) for new organofluorine drugs approved between January 1, 2020 and June 1, 2021 (KEGG, 2021). KEGG Drug Database is a publicly available repository of approved drugs in the U.S., Europe and Japan, their chemical properties, and molecular structure, and other identifiers for prescription and over-the-counter (OTC) pharmaceuticals, including organofluorine pharmaceuticals that have been withdrawn either due to lack of demand or risk to patients.

The organofluorine pharmaceuticals identified from the KEGG Drug Database were queried using PubChem for the drug names, available synonyms, CAS registry number, molecular structure, chemical formula, InChI key, and therapeutic use area (Kim et al., 2019). Drug name refers to the generic pharmaceutical name; available brand names the pharmaceutical is sold under are listed separately as synonyms. Where available, the most recently collected data from 2019 on the number of U.S. prescriptions and the rank order by frequency prescribed within a calendar year were compiled from the ClinCalc DrugStats database (ClinCalc DrugStats Database, 2019) and are presented in Table 4 in addition to being made available in an Excel worksheet (Data S1). Drug utilization data from ClinCalc DrugStats was generated via the Agency for Healthcare Research and Quality's most recent Medical Expenditure Panel Survey (MEPS) from 2019, accessed in January 2022 (Agency for Healthcare Research and Quality, 2019). MEPS is a large-scale nationally representative survey of households and medical care providers across the U.S. and includes information on household-reported prescription drug use.

We also compile data on global sales and revenues from PharmaCompass, where available, on the organofluorine pharmaceuticals that rank in the top 500 prescribed drugs (PharmaCompass, 2021). ''Blockbuster'' drugs are defined as those whose global sales exceed $1B annually. Revenues can change from year to year based on whether a drug's patent is expired, and the availability of generics. It is more useful and consistent with the available data to compare the total number of prescriptions in a calendar year as a measure of how widely a drug is used. The pharmaceutical name and CAS registry number refers to the non-ionic form of the drug, unless the ionic equivalent is necessary for identification in which case both forms are included. Ionic equivalents are presented primarily for corticosteroids in which case multiple ionic forms of the compounds have distinct clinical uses. For example, fluoxetine hydrochloride is presented simply as fluoxetine whereas fluticasone propionate and fluticasone furoate are presented separately since they are different drugs with unique pharmacological activity.

Quantitative and qualitative analysis

Each of the identified organofluorine pharmaceutical structures were reviewed against the nine definitions. The definitions were ranked from most to least inclusive with the most inclusive definition containing the largest number of compounds. We describe ambiguities in some definitions with examples.

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Article

Prevalence and Source Tracing of PFAS in Shallow Groundwater Used for Drinking Water in Wisconsin, USA

Matthew Silver,* William Phelps, Kevin Masarik, Kyle Burke, Chen Zhang, Alex Schwartz, Miaoyan Wang, Amy L. Nitka, Jordan Schutz, Tom Trainor, John W. Washington, and Bruce D. Rheineck*

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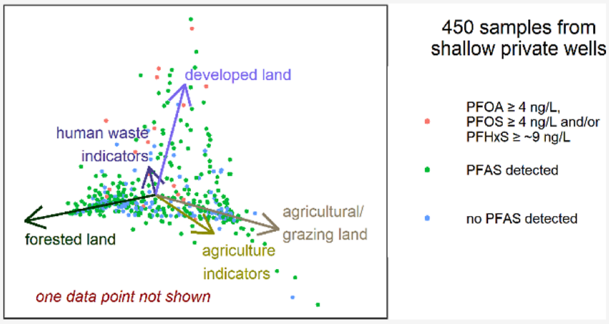
ABSTRACT: Samples from 450 homes with shallow private wells throughout the state of Wisconsin (USA) were collected and analyzed for 44 individual per- and polyfluoroalkyl substances (PFAS), general water quality parameters, and indicators of human waste as well as agricultural influence. At least one PFAS was detected in 71% of the study samples, and 22 of the 44 PFAS analytes were detected in one or more samples. Levels of PFOA and/or PFOS exceeded the proposed Maximum Contaminant Levels of 4 ng/L, put forward by the U.S. Environmental Protection Agency (EPA) in March 2023, in 17 of the 450 samples, with two additional samples containing PFHxS $\gtrsim$ 9 ng/L (the EPA-proposed hazard index reference value). Those samples above the referenced PFAS levels tend to be associated with developed land and human waste indicators (artificial sweeteners and pharmaceuticals), which can be released to groundwater via septic systems. For a few samples with levels of PFOA, PFOS, and/or PFHxS > 40 ng/L, application of wastes to agricultural land is a possible source. Overall, the study suggests that human waste sources, septic systems in particular, are important sources of perfluoroalkyl acids, especially ones with ≤8 perfluorinated carbons, in shallow groundwater.



KEYWORDS: *PFAS occurrence, emerging contaminants, human waste sources, septic system effluent, waste land application, agricultural sources, source water protection*

1. INTRODUCTION

Per- and polyfluoroalkyl substances (PFAS) are a large group of synthetic chemicals used in consumer, firefighting, and industrial products since the 1950s that pose a threat to drinking water supplies. In the past decade, environmental occurrence studies have found that PFAS occur ubiquitously in many environmental media, including treated wastewater,[1,2] surface water,[3,4] soil,[5,6] and precipitation.[7−9] In previous site- or region-specific investigations, PFAS have been found in groundwater, with concentrations varying over several orders of magnitude.[10] Groundwater is the source of about 39% of the water supplied by public water systems in the United States as well as the source of water for private wells, which are used by about 15% of the population.[11] Based on results from the U.S. Environmental Protection Agency's (EPA) Third Unregulated Contaminant Monitoring Rule (UCMR3) sampling of municipal water systems conducted in 2013−2015, it was estimated that drinking water supplies exceed the 2016 EPA Health Advisory Level of 70 ng/L PFOA + PFOS for ~6 million U.S. residents.[12] Incorporation of more recent data indicates that PFOA + PFOS in U.S. drinking water may exceed 1 ng/L for more than 200 million people in the United States.[13] In a recent survey of select groundwater aquifers used as a source of drinking water in the eastern United States, one or more PFAS were detected in 47% of 254 samples.[14] In March 2023, the EPA proposed[15] maximum contaminant levels (MCLs) of 4 ng/L for PFOA and 4 ng/L for PFOS, as well as a hazard index MCL goal that includes four additional PFAS.

Considering the importance of groundwater to drinking water supplies, more remains to be learned about the prevalence of PFAS, where they are found, and contributions from different sources. There are numerous potential types of sources of PFAS in groundwater. The source type that has received perhaps the most attention is aqueous film-forming foams (AFFFs), which are designed to be used on flammable liquid fires. AFFF discharges in training exercises and fire response are known to be

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NMOGA Exhibit D12

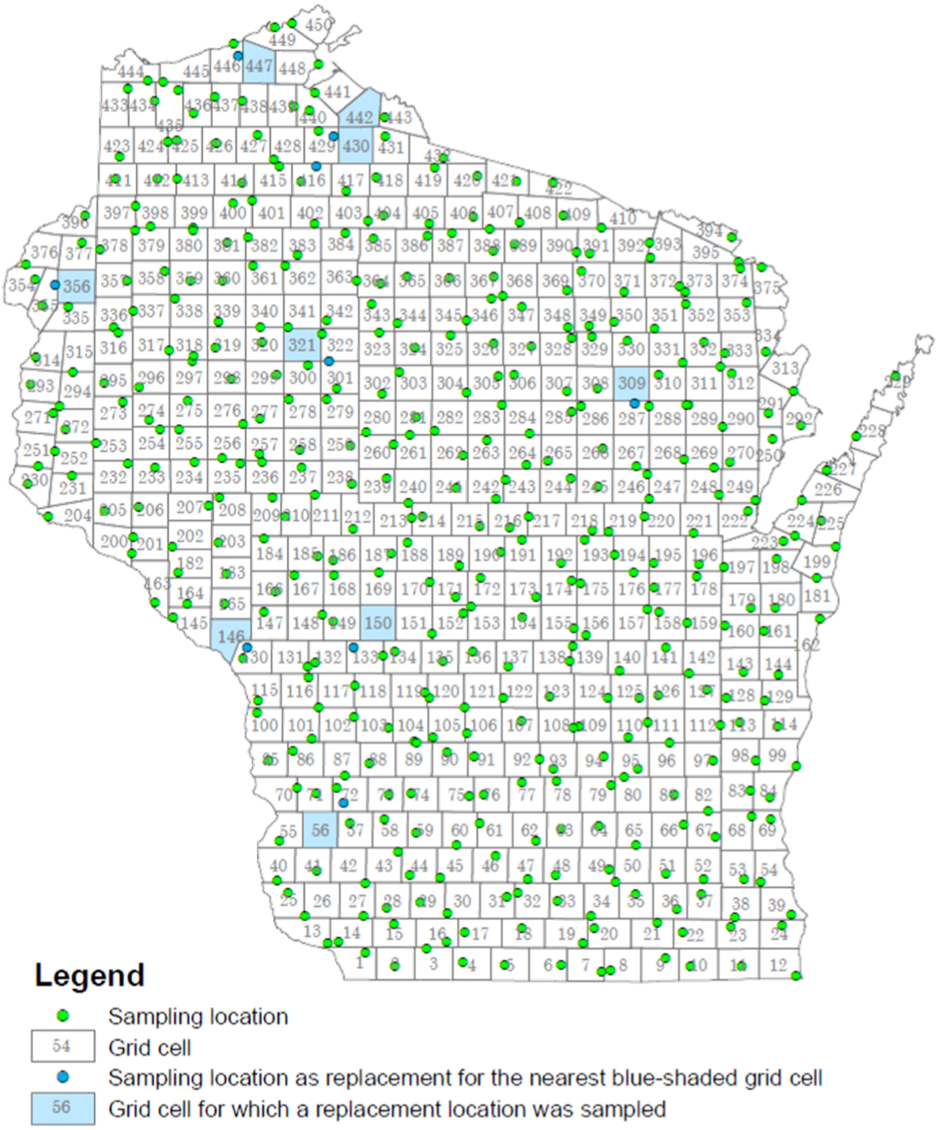

Figure 1. Grid cells and project sampling locations. Reproduced with permission from the Wisconsin Department of Natural Resources.

a means of contaminating groundwater.[16−19] Additionally, the presence of military sites in watersheds used for groundwater-sourced water supplies was found to increase the likelihood of municipal drinking water contamination.[12] AFFFs, landfills,[20] and industrial activities[12] (direct discharges) are among the most notable potential point sources of PFAS to groundwater. Potential nonpoint sources include precipitation (PFAS have been found in Wisconsin precipitation in the single digits of ng/L[9]) as well as PFAS-containing materials that can be land-applied, such as sewage sludge ("biosolids") from wastewater treatment plants,[12,21−23] septage (liquid and solid waste from septic systems, holding tanks, and/or portable restrooms), industrial wastes from the manufacture of consumer products, manure,[21] and pesticides.[24,25] While we are not aware of any studies documenting PFAS in septage, PFAS have been found in a variety of toilet paper products.[26] PFAS have also been found in household consumer products such as impregnation agents, paper, leather products, carpets, and other textiles and clothing.[27−31] Due to the common presence of these product types in households, another possible source of PFAS in groundwater is septic system (onsite wastewater treatment system) effluent. Two previous studies performed in areas with many private wells and septic systems found indications that septic systems may be a source of PFAS in groundwater.[32,33] Once released on or near the land surface, PFAS are known to accumulate at air−water interfaces,[34,35] which are abundant in unsaturated zone soil, leading to an observed tendency to find higher concentrations at shallower subsurface depths.[16,36,37] Other factors that can potentially influence the occurrence and transport of PFAS in the subsurface include sorption,[38,39] generally with higher sorption of perfluoroalkyl sulfonic acids (PFSAs) compared to perfluoroalkyl carboxylic acids (PFCAs),[40,41] and the tendency for more sorption with longer perfluoroalkyl carbon chain length.[41,42]

In this study, we characterized the prevalence of PFAS in Wisconsin's ambient shallow groundwater using an Equal Area Grid[43,44] approach that included collection of 450 water samples from residences with private wells. "Ambient" refers to locations at least three miles away from sites related to previously known PFAS releases where regulatory actions are pending or have already been taken. For the purposes of this study, "shallow" groundwater is considered to be groundwater from the uppermost 40 feet of the uppermost continuous local aquifer. The sample size of 450 was chosen in consideration of previous surveys of Wisconsin groundwater for agricultural chemicals,[45] which utilized about 400 samples statewide as the minimum number needed to statistically characterize groundwater impacts. Our study is similar to that of McMahon et al.[14] in use of a suite of water quality parameters in addition to PFAS and an Equal Area Grid approach to well selection but also differs in a few ways, most notably well type and depth. McMahon et al.[14] sampled networks that are mostly (64%) public wells, while we sampled only shallow (as defined above) private wells.

The objective of this study was to provide a snapshot in time of the current prevalence of PFAS in shallow groundwater across Wisconsin and to better understand the levels and major source types of PFAS in groundwater, which is the source of drinking water for approximately 70% of Wisconsin residents (public and private wells combined). Sampling shallow private wells allows characterization of the quality of drinking water currently being consumed by many private well owners and is analogous to the roughly 10,000 small public systems' wells in the state, while also enabling an improved assessment of the susceptibility of deeper groundwater supplies (which are utilized by many larger public water systems and deeper private wells) to contamination. We also utilize land use data to make inferences on the contributions of potential types of sources of PFAS to groundwater and identify risk factors for higher concentrations of PFAS in shallow private wells. To aid in identification of dispersed human waste sources in this study, water samples collected from homes with private wells were analyzed for two indicator suites, based on Nitka et al.:[46] artificial sweeteners (acesulfame and sucralose) and pharmaceuticals (carbamazepine and sulfamethoxazole) as human waste indicators (HWIs) and metabolites of two commonly used herbicides (alachlor and metolachlor) as indicators of agricultural activities.

2. MATERIALS AND METHODS

2.1. Sample Point Selection. Study sampling locations were selected in three steps. In Step 1, based on the Equal Area Grid methodology,[44] Wisconsin was divided into 450 grid cells of equal area, with a target area of 321 km^2 (124 square miles) (Figure 1). In Step 2, lists of private water supply wells in each of the 450 grid cells meeting the following criteria were compiled: (1) a Well Construction Report (WCR) is available, and (2) casing extends downward at least to the static water level noted on the WCR but no deeper than 40 ft below the static water level. The purpose of these criteria was to sample water from homes with wells drawing relatively shallow groundwater and casing that prevents contributions from the vadose zone, enabling comparability of results across the state. In order to investigate PFAS in ambient groundwater, WCRs for locations within three miles of an existing Wisconsin Department of Natural Resources (DNR) site with actionable PFAS concentrations (as of April 22, 2022) were excluded. A large enough radius to provide an amount of safety for avoiding wells affected by a source subject to regulatory action was desired, but with typical grid cell widths around 11.1 miles, excluding areas larger than a circle with a three-mile radius would have risked excluding too many wells within a single grid cell. Additional details, including recruitment of participants with candidate private wells in Step 3, are described in the Supporting Information.

2.2. Sampling. Water samples were collected from a home plumbing system tap connected to a home's water supply well. Before sampling, information provided by the homeowner/resident(s) about the presence of any treatment system was reviewed. The default sampling location was an outdoor faucet; however, if the homeowner/resident(s) indicated treatment was installed, adjustments (e.g., different tap or temporarily bypassing the treatment system) were made as necessary to sample untreated water.

Sampling was performed by trained teams of two samplers, following the procedure detailed in Section S1.1 of the Supporting Information. Briefly, water was purged until temperature, conductivity, and pH stabilized. After stabilization, water flow was turned down, then the primary sampler put on nitrile gloves, filled two 250 mL polypropylene (PP) bottles, and collected a PFAS field blank at every site by pouring laboratory-provided water into an empty 250 mL PP bottle. Following the collection of PFAS samples, additional sample bottles for non-PFAS laboratory analysis were filled. Further details on sample bottles and field QC samples are provided in Supporting Information.

2.3. PFAS Lab Analysis. PFAS standards were purchased from Wellington Laboratories and Cambridge Isotope Laboratories. Analytes and extracted internal standards are listed in Tables S1 and S2. Blank water (18.2 MΩ·cm resistivity) with no detectable PFAS levels was generated by an ELGA water purification system.

Extraction and analysis for PFAS (see Table 1 for a list of analytes detected and the Supporting Information for analytes without any detections) were conducted at the Wisconsin State Laboratory of Hygiene based on the ISO 21675[47] draft method. Aqueous samples were extracted using WAX SPE cartridges and analyzed using high-performance liquid chromatography tandem mass spectrometry (HPLC-MS/MS) in negative ion mode. Analyte concentrations were quantified using isotope

Table 1. Analytes Detected in This Study and Method Detection Limits

analyte name (acid form)	analyte acronym	CAS number	detection limit (ng/L)
6:2 fluorotelomer sulfonic acid	6:2FTS	27619-97-2	0.257
perfluorobutanoic acid	PFBA	375-22-4	0.327
perfluoropentanoic acid	PFPeA	2706-90-3	0.142
perfluorohexanoic acid	PFHxA	307-24-4	0.193
perfluoroheptanoic acid	PFHpA	375-85-9	0.142
perfluorooctanoic acid	PFOA	335-67-1	0.102
perfluorononanoic acid	PFNA	375-95-1	0.140
perfluorodecanoic acid	PFDA	335-76-2	0.154
perfluoroundecanoic acid	PFUnA	2058-94-8	0.210
perfluorododecanoic acid	PFDoA	307-55-1	0.256
perfluorotridecanoic acid	PFTrDA	72629-94-8	0.183
perfluorotetradecanoic acid	PFTeDA	376-06-7	0.166
perfluoropropanesulfonic acid	PFPrS	423-41-6	0.244
perfluorobutanesulfonamide	PFBSA	30334-69-1	0.409
perfluorobutanesulfonic acid	PFBS	375-73-5	0.219
perfluoropentansulfonic acid	PFPeS	2706-91-4	0.129
perfluorohexanesulfonic acid	PFHxS	355-46-4	0.134
perfluoroheptanesulfonic acid	PFHpS	375-92-8	0.180
perfluorooctanesulfonic acid	PFOS	1763-23-1	0.135
perfluorooctanesulfonamide	PFOSA	754-91-6	0.147
N-ethyl perfluorooctane sulfonamidoacetic acid	NEtFOSAA	2991-50-6	0.201
perfluoro(perfluoroethyl) cyclohexanesulfonic acid	PFECHS	133201-07-7	0.181

D12.4

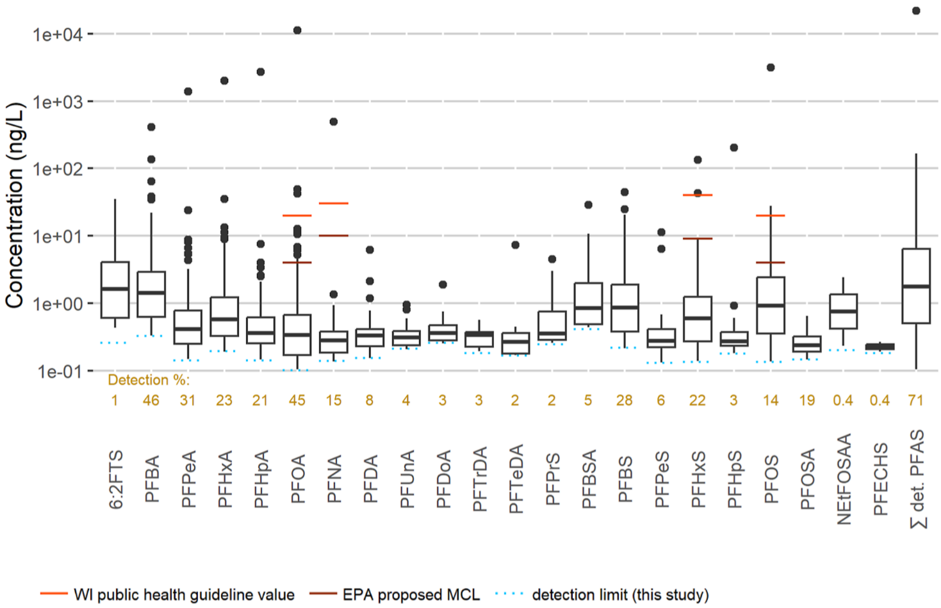

Figure 2. Prevalence of PFAS detected in the 450 samples (for acronyms, see Table 1). The percentage of samples with detections is shown above the compound names, while the boxes, whiskers, and points display the detected concentrations. Boxes show the 25th through 75th percentile concentrations, while whiskers (lines no greater than 1.5 times the length from the 25th to 75th percentile) and black dots combined show detected concentrations outside of the 25th through 75th percentiles. The $\sum$ det. PFAS variable is the sum of any PFAS that were detected in each sample.

dilution for those analytes with an existing commercially available exact isotopically labeled standard. Analytes for which there was no commercially available exact isotopically labeled standard were quantified using extracted internal standards (isotopically labeled) of chemically similar compounds, close in retention time to the native analyte. For compounds with commercially available qualitative or quantitative standards containing branched and linear isomers, the PFAS analyte was reported as a single analyte consisting of the total amount of linear and branched isomers. Additional method details are provided in the Supporting Information.

2.4. Non-PFAS Lab Analysis. Compounds indicative of human waste and agricultural impacts were analyzed to aid in contaminant source tracing. The following four HWIs were analyzed: acesulfame (artificial sweetener), sucralose (artificial sweetener), carbamazepine (antiepileptic), and sulfamethoxazole (human antibiotic pharmaceutical). Additionally, four chloroacetanilide metabolites (CAAMs), alachlor ethanesulfonic acid (ESA), alachlor oxanilic acid (OA), metolachlor ESA, and metolachlor OA (for structures, see Supporting Information, Figure S1), were chosen as indicators of agricultural impacts. The parent compounds (alachlor and metolachlor) have commonly been used on corn and soybeans in Wisconsin[45,48] (corn and soybeans are the largest crops in Wisconsin by harvested acreage[49]). The metabolites are more polar and therefore more likely to be detected in groundwater than their respective parent compounds.[50]

HWIs and CAAMs were analyzed at the University of Wisconsin−Stevens Point's Water and Environmental Analysis Laboratory (WEAL). Site samples and quality control samples were prepared for analysis using solid-phase extraction. Extracts were analyzed using liquid chromatography tandem mass spectrometry with an electrospray ionization source (LC-ESI/MS/MS). Analysis for HWIs was adapted from EPA Method 1694 and Nitka et al. (2019). CAAM analysis was adapted from Zimmerman et al.[51] Methods and standards are detailed in the Supporting Information.

2.5. Statistical and Spatial Data Analysis. Statistical analysis was performed using R for Windows version 4.3.0 (The R Foundation for Statistical Computing). Box-and-whisker plots were generated directly from all detected concentrations. For representing study sites by land use type, land use for circular areas around wells was compiled from Wiscland2,[52] utilizing a 500 m radius, which was validated by a USGS study[53] that evaluated different sizes and geometries for approximating the capture zone to a well. After the compilation of land use for each well, proportionality tests were then used to compare PFAS detection rates across land use categories. Specifically, for those proportionality tests, we first classified each sample as either PFAS detected (at any concentration) or no PFAS detections and then used the R function "prop.test", which calculates p-values based on the chi-squared statistics under the null hypothesis of equal PFAS detection rates. Next, differences in PFAS concentrations grouped by land use type were tested using two-sample Mann-Whitney-Wilcoxon nonparametric rank sum tests after first recensoring the sum of detected PFAS by replacing any values (detected or not) below the highest detection limit of any PFAS analyte (0.409 ng/L) with 1/10th of that value (adapted from Section 5.1 of Statistical Methods in Water Resources[54]). Finally, for the generation of Spearman correlation coefficients and principal component analysis, results below the highest detection limit for each compound were recensored to 1/10th of the compound-specific detection limit (Table 1). A matrix of Spearman correlation coefficients was produced using the R function "cor" and corrected for family-wise significance following Holm's sequential procedure.[55] Principal component analysis was performed using the R function "prcomp", including scaling of all variables before generating the principal components.

3. RESULTS AND DISCUSSION

3.1. Occurrence. At least one PFAS was detected in 71% of the 450 samples (Figure 2). PFBA was the most frequently detected compound (46% of samples), followed by PFOA (45%

of samples). Since there is a higher detection limit for PFBA than PFOA (Table 1), the relative prevalence of PFBA in groundwater may be much higher than PFOA (discussed further in the next paragraph). For PFOA, three sample results are above the 2019 Wisconsin Department of Health Services public health value of 20 ng/L and 13 are above the March 2023 EPA proposed MCL of 4 ng/L. For PFOS, two are above the Wisconsin public health value of 20 ng/L and 11 are above the EPA proposed MCL of 4 ng/L. PFHxS results for two samples are above both the Wisconsin public health value and the EPA proposed MCL Health Based Water Concentration (40 and 9 ng/L, respectively). Overall, four of the 450 study samples (1%) had one or more PFAS above a Wisconsin public health value, and 19 of the 450 (4%) had one or more PFAS above an EPA proposed MCL (including Health Based Water Concentrations). The 71% rate of detection of one or more PFAS in this study, in which we exclusively sampled wells with relatively shallow casing, is higher than the 45% rate suggested by modeling in a recent U.S.-wide study with a different set of sample types.[56]

Because detection limits vary by analyte (Table 1), some compounds in Figure 2 are censored at higher levels than others. To compare all compounds starting from the same minimum level, Figure S2 presents boxplots with a minimum comparison level for all compounds at 0.181 ng/L, corresponding to the median detection limit of all 22 detected compounds. For three compounds, concentrations modeled below the compound-specific detection limit using regression on order statistics[57,58] (ROS) are included. ROS was performed for all detected compounds, with only PFBA, PFDoA, and PFBS having modeled concentrations (plots in Figure S3) at or above 0.181 ng/L. At least one PFAS was detected at ≥0.181 ng/L in 65% of the study samples. Among PFCAs, inferred prevalence peaks at C4 (PFBA, also the most prevalent PFAS overall) and decreases with each increase in chain length through C7 (PFHpA, detected at ≥0.18 ng/L in 19% of the study samples). Prevalence rises again at C8 (PFOA, detected at ≥0.18 ng/L in 32% of the study samples) and then also decreases with increasing chain length through C14 (PFTeDA, detected at ≥0.18 ng/L in 2% of the study samples). For PFSAs, (inferred) detection frequencies are higher for even chain lengths, and among even chain lengths, detected or modeled prevalence ≥0.181 ng/L decreases with chain length: PFBS 29%, PFHxS 20%, and PFOS 12%. ROS modeling was performed for these comparisons of prevalence only; ROS-modeled concentrations are not used further.

While the analyte list consists of 16 precursors of perfluoroalkyl acids (PFAAs, which are combinations of the PFCA and PFSA groups), only four precursors were detected: 6:2FTS, a precursor of PFHxA and other short-chain PFCAs; PFBSA, a precursor of PFBS; PFOSA, a precursor of PFOS; and NEtFOSAA, also a precursor of PFOS. Boxplots of non-PFAS analytes/parameters are shown in Figures S4 and S5.

While the study sampling locations were selected to be representative of ambient groundwater, one sample had PFOA detected at 11,300 ng/L and eight other PFAS detected at concentrations above 100 ng/L. This occurred despite a sampling location selection process that excluded areas within three miles of a previously known site with actionable PFAS concentrations. In order to have actionable PFAS concentrations, compelling evidence of a local discharge is necessary. The fact that these levels were found, despite our site selection process avoiding previously known contamination, points to the possibility that other locations in Wisconsin with PFAS discharges capable of creating a hazard to public health may exist but had not yet been identified and/or subjected to regulatory actions at the time of the study. Additional sampling, driven by the need to protect public health, of water from other homes with private wells in a three-mile radius from the original study site (i.e., the one with the PFOA result of 11,300 ng/L) has found at least 31 additional locations with PFOA above 1000 ng/L (all samples were analyzed by Wisconsin DNR-certified laboratories using EPA Method 537.1 or a laboratory-specific isotope dilution method that meets Wisconsin DNR PFAS method expectations[59]). This site is discussed further at the end of Section 3.2.

3.2. Source Tracing. PFAS occurrence in groundwater may be affected by many factors. For lower concentrations, this includes the ubiquitous detection of PFAS in precipitation.[7−9] There are 57 samples from this study (Figure S6) for which all detected PFAS were at or below the highest site median from a Wisconsin precipitation study[9] with sample collection (91 samples from eight sites mostly reflecting ambient conditions) during 2020. Detected PFAS in the 57 samples (this study) were the C4−C9 PFCAs, PFTeDA, PFHxS, PFOS, and PFOSA. Identification of these PFAS and their levels in our study samples serves as an estimate of which PFAS in groundwater could have come from precipitation plus dry deposition, without elevated levels from discrete sources. Uncertainties in this estimate include that PFAS may accumulate in soils before breakthrough to groundwater[5,60] and that historical levels in precipitation are largely unknown.

Differences in land use could affect PFAS occurrence at any concentration. Figure 3 shows prevalence comparisons by land use (Wiscland2[52]), with samples categorized by the highest percentage of land use in the 500 m circle around each well. Figure 3a displays PFAS detection rates across these categories, with the highest detection rate in the developed category. Proportionality tests show significant differences between developed areas (reflecting housing density) vs other categories

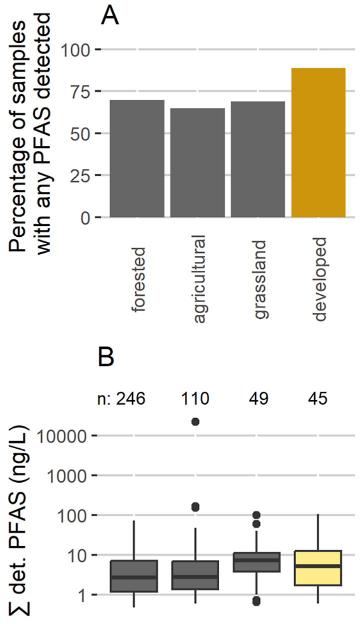

Figure 3. (A) Rates of PFAS detection by the largest land use type within 500 m of each sample location (see B for number of samples per category) and (B) boxplots of the sum of detected PFAS, where one or more was detected.

D12.6

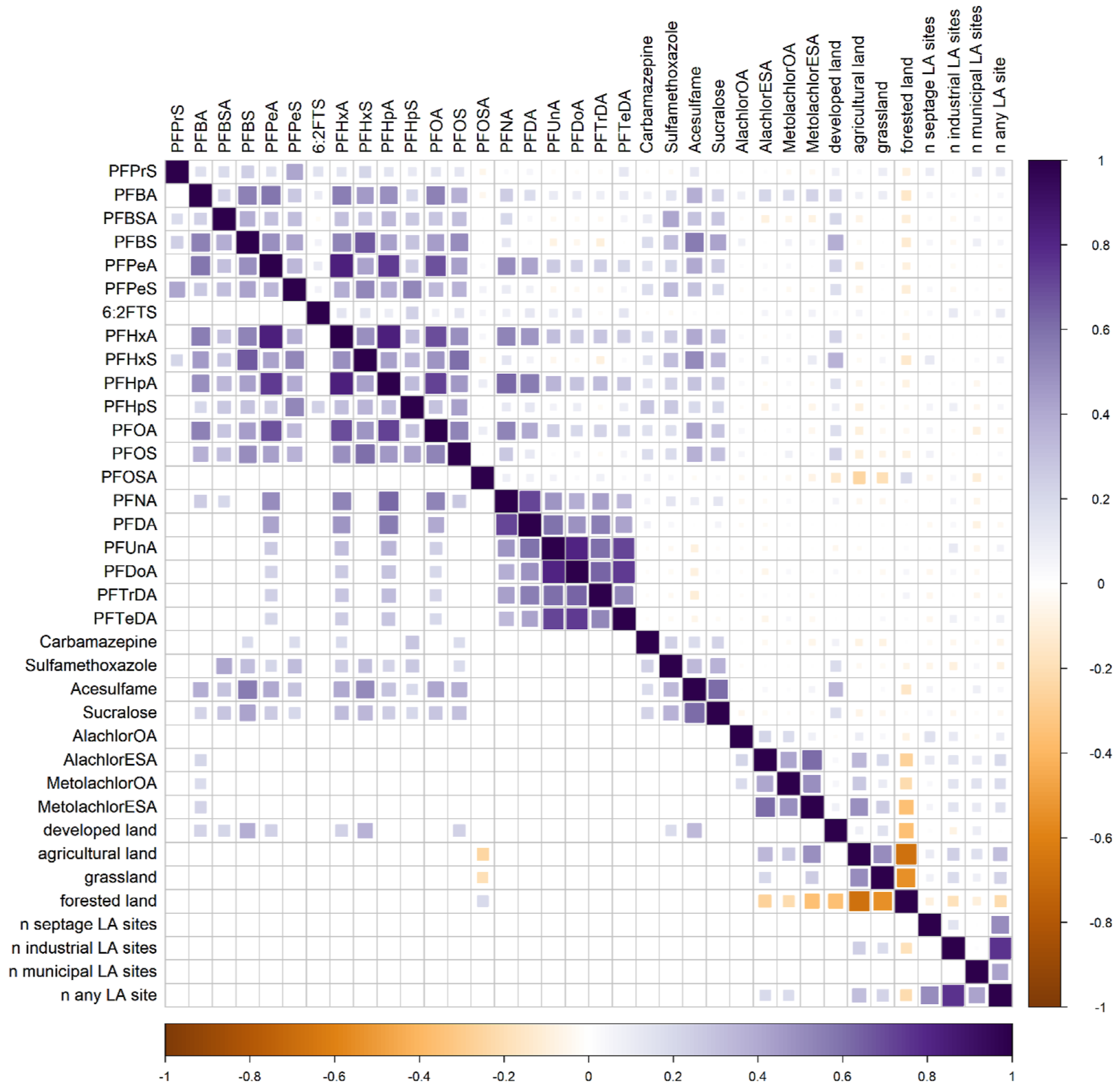

Figure 4. Correlation plot with intensity and amount of color indicating the value of the Spearman correlation coefficient (ρ) between variable pairs. The upper-right triangle shows all correlation values, regardless of p-values, while the lower-left triangle shows colored squares only for significant correlations (Holm sequentially adjusted $p < 0.05$).

(developed vs forested, p = 0.02; developed vs agricultural, p = 0.004; developed vs grassland, p = 0.04), suggesting that PFAS detections are more likely to occur in developed areas. Compound-specific detection frequencies (Figure S7) show that developed vs forested and developed vs agricultural differences are driven largely by detection rates of the C4−C7 PFCAs, PFBSA, and the C4−C8 PFSAs (except for PFHpS). Figure 3b shows, for samples with detection of one or more PFAS, box-and-whisker plots of the sum of all detected PFAS in each sample across the land use categories (for detection rate, see Figure 3a). The median values of $\sum$ det. PFAS are slightly higher in developed land than both forested and agricultural areas. To incorporate the magnitude of detected concentrations into two-sample Mann-Whitney-Wilcoxon nonparametric rank sum tests, data were prepared as described in Section 2.5. These rank-sum tests indicate that PFAS levels in areas with "developed" as the largest land use are significantly different from levels in both the forested ($p = 7 \times 10^{-6}$) and agricultural ($p = 4 \times 10^{-4}$) categories (comparison of developed to grassland gives an approximate—due to ties in rank—p-value of 0.02). These tests indicate that both detection rate and $\sum$ det. PFAS levels are higher in developed areas. However, it is also noteworthy that four of the five highest $\sum$ det. PFAS levels are in areas with either agriculture or grassland as the main land use. Land application of wastes is a possible source of PFAS in groundwater.[22,61] While ∼18% of the study sampling sites in both the forested and developed categories had land application of wastes in proximity to the sampling site, that percentage is 37% for grassland (including land used for livestock forage production and grazing; see Supporting Information, Section S1.5, for more information) and 49% for agricultural land.

Figure 4 shows Spearman ρ correlations between many study variables (additional variables are shown in Figure S8), including land use and the number of nearby waste land application sites (radius of 1000 m, reflecting the 500 m radius used for land use plus a buffer for waste application point location inaccuracies).

Colors and square sizes in Figure 4 reflect the magnitude of the Spearman ρ value. Because Figure 4 depicts 630 comparisons, a small fraction of the "significant" results in this large number of comparisons could arise from chance alone. Thus, while the upper-right triangle of Figure 4 shows all Spearman ρ correlations, the lower-left triangle of Figure 4 only shows correlations that are family-wise significant at $\alpha = 0.05$ after Holm sequential adjustment[55] (for those Holm sequentially adjusted p-values, see Table S24). Where multiple contiguous PFAS homologues load significantly on a single independent variable, this outcome provides more robust evidence of a causal factor. In contrast, lone "orphan" significant comparisons may, in some cases, arise by chance. Among PFAS, a grouping of shorter chain compounds (from PFPrS through PFOS, with the exception of 6:2FTS) mostly shows significant positive correlations with each other. For example, PFHxA shows strong (Spearman $\rho > 0.49$) correlations with PFBA, PFBS, PFPeA, PFHxS, PFHpA, PFOA, PFOS, and PFNA (p-values for the named are all lower than 10^{-25}). PFOA shows moderate (Spearman $\rho > 0.19$) to strong correlations with all other PFCAs except PFTeDA, with Spearman ρ values ranging from 0.19 (PFTeDA, $p = 5 \times 10^{-3}$) to 0.72 (PFHpA, $p = 2 \times 10^{-71}$). One notable pair is PFOA and PFNA (Spearman $\rho = 0.53$, $p = 2 \times 10^{-31}$), both of which can be a product of 8:2 FTOH degradation in the atmosphere.[62] Combined with degradation studies,[63−66] this suggests the possibility of a common fluorotelomer origin for those compounds. Among C10−C14 PFCAs, correlations to C8 and shorter chained PFSAs and PFBSA are sparse.

The compounds PFBS and PFBSA show moderate to strong correlations with the HWIs acesulfame, sucralose, and sulfamethoxazole (lowest Spearman ρ is PFBSA to sucralose at 0.28, $p = 7 \times 10^{-7}$). PFOSA is the C8 homologue of PFBSA (C4) and PFOSA is known to transform in the environment to PFOS,[2] making PFBSA a suspected PFBS precursor. Previous studies have shown that legacy pre-2002 electrochemical fluorination AFFFs contain PFBS (and possible PFBS precursors),[17,18,67,68] while one commercial product that has been found to contain PFBSA is "Scotchgard" produced after 2002[69] (the latter could result in the presence of PFBSA in clothing and other household sources). In two studies of precipitation,[8,9] PFBS was analyzed but not detected in any samples. Both legacy (produced before ∼2002) AFFFs and post-2002 Scotchgard product are possible sources of PFBS and PFBSA in shallow groundwater.[67] The significantly higher (see Table S24 for p-values) prevalence of PFBS and PFBSA in samples from the developed land use category (Figure S7) and the correlations with acesulfame, sucralose, and sulfamethoxazole point toward human waste sources (septic system effluent; land application of septage or biosolids) as important ones to account for PFBS and PFBSA in shallow groundwater.

In the order the PFAS are listed in Figure 4, the compounds PFBA through PFOS (with the exceptions of 6:2FTS overall and sulfamethoxazole to PFBA and PFOA) show significant correlations with the HWIs sulfamethoxazole, acesulfame, and sucralose (among those pairs, the least significant correlation is for PFOS-sulfamethoxazole at $p = 4 \times 10^{-2}$). Significant correlations with developed land (represented as a decimal for the portion of land use in 500 m around the well) are present for several of those same PFAS (specifically, PFBA, PFBSA, PFBS, PFPeA, PFHxA, PFHxS, and PFOS), with the lowest Spearman ρ among these pairs being with PFBSA, with Spearman $\rho = 0.21$ ($p = 2 \times 10^{-3}$). The positive correlations between these PFAS and HWIs are an indication that human waste sources may play an important role in PFAS occurrence. This is similar to the findings of Schaider et al. that suggested that septic systems are a likely source of PFAS in private wells.[32] Our study, however, includes a wide variety of land uses and activities, such as land application of biosolids and septage, which may also be PFAS sources. The presence of PFAS in biosolids, at varying concentrations, is well documented;[21,22,70] however, we are not aware of any studies documenting PFAS levels in septage.

The HWIs chosen for this study can be useful in identifying influence from human waste sources, especially in agricultural areas where contributions from land-applied wastes are minimal.[46] However, in addition to samples from septic systems,[71,72] the HWIs have also been found in biosolids,[73,74] making them nonunique tracers among dispersed human waste sources. While HWIs can be present in landfills[75] (another dispersed source of human wastes), acesulfame and sucralose were approved by the U.S. Food and Drug Administration between 1988 and 1999,[76] making it unlikely that they are associated with historic landfill sources. The solid−liquid partitioning behavior of HWIs in wastewater treatment (including septic systems) may reflect where the most mass loading to the environment occurs. On the one hand, acesulfame and sucralose are highly water-soluble[77] and have been found in wastewater effluent at levels ∼50 times higher than sludge.[77,78] On the other hand, sulfamethoxazole and carbamazepine have activated sludge sorption coefficients (K_d) of 9.7 and 91 L/kg, respectively,[79] indicating strong partitioning to sludge (biosolids) rather than wastewater. Sulfamethoxazole has been detected in private wells on Cape Cod, with septic systems being a likely source.[80] Since discharge to groundwater from a septic system can readily result in high concentrations of mobile compounds such as artificial sweeteners and many short-chain PFAAs, and also considering the higher PFAS correlations with developed land than agricultural land, septic systems can be viewed as a likely source of PFAS in groundwater. However, other human waste sources cannot be ruled out as possibly contributing some of the PFAS to groundwater.

PFBA was detected at significantly higher concentrations in an area of western Wisconsin (Figure S9) compared to the rest of the state (two-sample nonparametric rank sum test $p = 8 \times 10^{-12}$). The water solubility of PFBA has been estimated to be 2 orders of magnitude higher than that of PFOA[81] and higher sorption of PFOA compared to PFBA has been found,[38,82] suggesting relatively high mobility of PFBA in groundwater. While definitive attribution of the source(s) and transport mechanism(s) of the higher PFBA levels in western Wisconsin shallow groundwater is beyond the scope of this study, it is noteworthy that PFBA has been found as the predominant PFAS compound in some impacted environmental waters to the west in Minnesota.[83,84] High PFAS levels in soil samples in major downwind directions of factories using or manufacturing PFAS have been found in New York/Vermont[85] and New Jersey,[86] suggesting that aerial contamination can contaminate soil downwind of a major source. The New York/Vermont study additionally attributed groundwater PFOA contamination to that pathway.[85]

Of the CAAM analytes, three are significantly correlated with PFBA, but no other significant relationships are found between CAAMs and PFAS (Figure 4). PFBA was among the most frequently detected PFAS in Wisconsin precipitation[9] and is the most frequently detected PFAS in this study (Figure 2). While there are a variety of possible sources of PFAS in agriculture,[87]

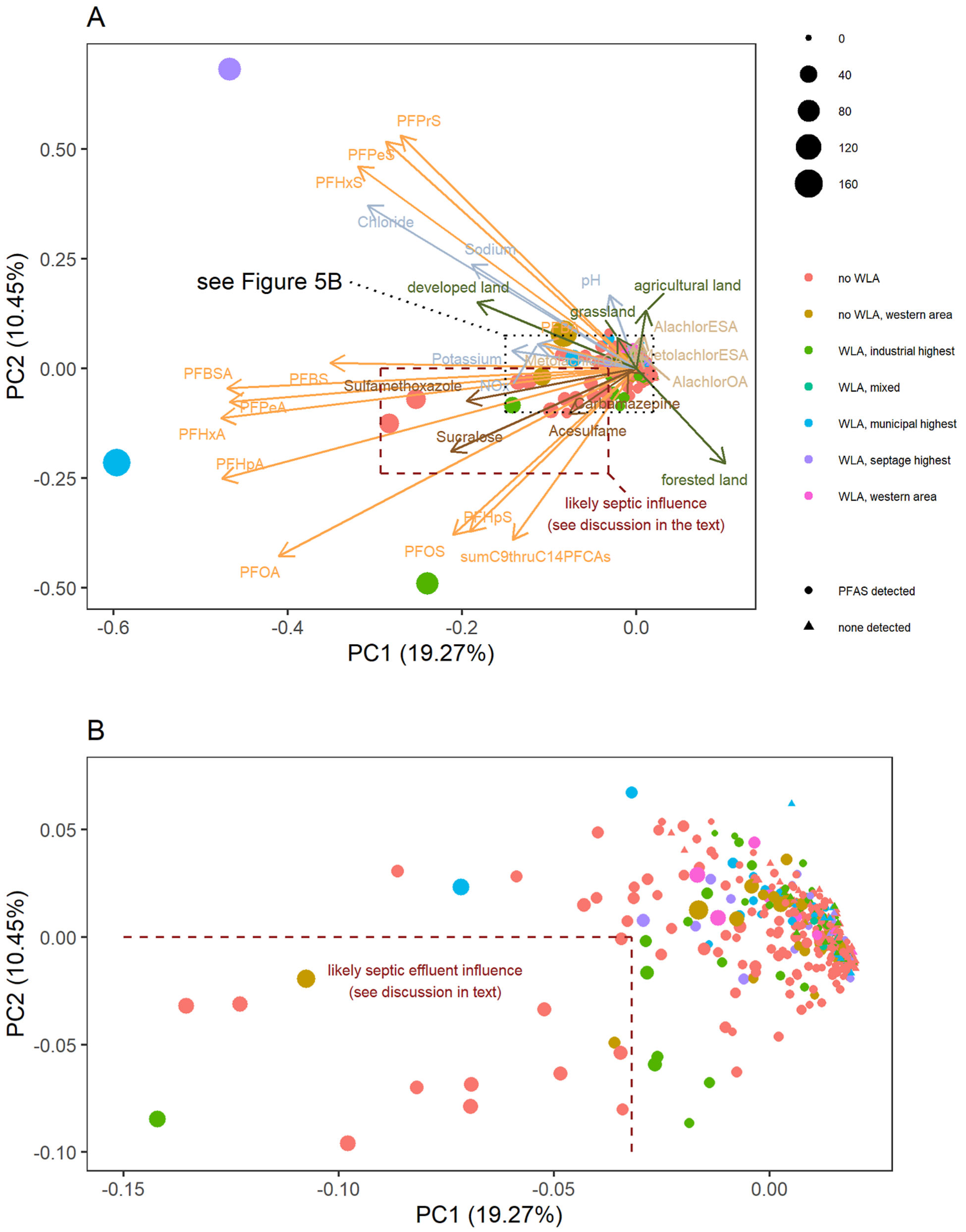

Figure 5. Principal component analysis plots for all samples (A) and zoomed in on a smaller area (B), which is indicated by the block dotted rectangle on (A). Symbol shape indicates whether PFAS were detected, and symbol size is proportional to the sum of detected PFAS. Colors of symbols indicate if waste land application (WLA) has been permitted nearby and also indicate which samples are located in the western area with higher PFBA concentrations.

there are no significant positive correlations between PFAS analytes and agricultural land use (Figure 4). The lack of significant correlations between the CAAMs and PFAS, other than three CAAMs with PFBA (discussed further below), suggests a limited relationship between CAAMs and PFAS. PFBA in western Wisconsin (Figure S9) could be from a nonagricultural source (e.g., precipitation, possibly with higher historical PFAS levels), and this raises the question of how much those western Wisconsin samples influence the correlations of PFBA with the three CAAMs showing significant correlations (Figure 4). With the 40 western Wisconsin (Figure S9) samples removed, the Spearman ρ correlation of PFBA with the three CAAMs with which PFBA has significant correlations ($p < 0.05$) decreases as follows: 0.22 to 0.13 for alachlor ESA, 0.22 to 0.17 for metolachlor ESA, and 0.19 to 0.18 for metolachlor OA. These comparisons are another indication, to the extent that it is viewed as likely that the higher PFBA in the area of western Wisconsin is attributable to something other than agriculture, of a limited role of agricultural land use on overall PFAS occurrence.

Principal component analysis (Figure 5) was performed on the results of 449 samples (the sample with PFOA at 11,300 ng/L is excluded). While waste land application is not the only diagnostic of the PFAS source for an individual sample, it can be informative to the source type where samples cluster. The area of the dark red dashed rectangle (Figure 5a) encloses the end of the loading vectors of three of the HWIs (acesulfame, sucralose, and sulfamethoxazole). Most of the samples in this region have no nearby waste land application, leaving septic system effluent as a likely source for most of these samples (and possibly also others closer to the plot origin in the same direction as those loadings). Stacked column plots showing the PFAS signatures (combinations of detected compounds) for the 19 samples with PFAS levels above the March 2023 EPA proposed MCLs are shown in Figure S10.

The loading vectors of PFPrS, PFPeS, and PFHxS, as well as those of developed land, chloride, and sodium, share a similar angular direction. A source other than septic systems (possibly legacy AFFFs) is likely for samples in that direction, though unlike within the dark red dashed box, there are few samples at moderate loading values in this angular direction. Three outliers are visible in Figure 5a. The sample toward the upper left had PFHxS detected at 42.6 ng/L. While the data point is colored in the septage land application category, there are also industrial sites in the area (in addition to the possibility of an AFFF source, although no PFOS was detected). For the outlying data points in the lower left and lower central portions of Figure 5a, no industrial sites are located nearby. Of these three outliers, the latter two (i.e., ones with negative values of PC2) can be viewed as having a higher likelihood of PFAS contamination from a waste land application source. While waste land application is a suspect for source attribution of those two outliers, the loading vectors of agricultural land and the four agricultural indicator compounds suggest that most agricultural practices are not a major source of PFAS in groundwater.

Figure 5 omits the sample with PFOA detected at 11,300 ng/L. The well for that sample is located near agricultural fields that have received biosolids, septage, and paper mill sludge. This raises the possibility of waste land application as the source. Investigation into the source(s) of the groundwater contamination in the area is part of a DNR-led site investigation that commenced in January 2023.

3.3. Implications for Source Water Protection. This study was done to characterize current levels of PFAS in Wisconsin's shallow groundwater, water that approximately 70% of the state's population currently uses as their drinking water supply. Furthermore, what is shallow groundwater today will typically move deeper over time, with the potential for PFAS to increasingly become a drinking water quality issue for municipal water systems that draw water from deeper high-capacity wells. Several lines of evidence point to human waste sources as contributors of PFAS to groundwater, with effluent discharged from septic systems likely a major source of PFAS in groundwater. Detected PFAS were generally low overall compared to the March 2023 EPA proposed MCLs, but 19 samples (4%) had levels above those of the proposed MCLs. Aside from the five samples with the highest $\sum$ det. PFAS, septic systems are a likely source for most of the other 15 samples above the EPA proposed MCLs. This study points to the importance of reducing PFAS in septic system wastewater streams and the need for more effective technologies and management strategies for these waste streams in order to protect drinking water supplies.

Results presented here also illustrate a different character of the PFAS problem for developed versus agricultural communities. Owners of shallow wells in developed areas can expect a greater likelihood that PFAS are present in their water supply at currently detectable levels. On the other hand, although the majority of agricultural and other lower population density locations have a lower likelihood of PFAS detection, a few samples with especially high PFAS levels were from locations with either agriculture or grassland as the highest land use. Absent characterization of wastes and utilization of that information in determining which wastes are applied to agricultural land, potable wells in agricultural settings that received land application of wastes would, from a cautious perspective, need to be regarded as having a high risk of containing especially high PFAS levels.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.est.3c02826.

Additional details related to sampling design, laboratory materials and methods, land use data set, prevalence with a minimum comparison level and ROS-modeled concentrations, non-PFAS field and lab parameters, comparison to Wisconsin 2020 PFAS precipitation levels, individual PFAS by land use category, expanded correlation plot, PFBA map, and stacked column plots for PFAS composition of project samples above EPA March 2023 proposed MCLs (PDF)

Additional tables detailing land use around each of the study wells, field parameters, lab results for all primary samples and field quality control samples, and Holm-adjusted *p*-values for the comparisons shown on Figure 4 (XLSX)

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Notes

The authors declare no competing financial interest.

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The Fifth Unregulated Contaminant Monitoring Rule (UCMR 5) Data Summary: July 2024

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July 2024
Office of Water (MS-140)

NMOGA Exhibit D13

Overview

The U.S. Environmental Protection Agency has released the fifth set of data collected under the fifth Unregulated Contaminant Monitoring Rule (UCMR 5) for the 30 chemical contaminants (29 per- and polyfluoroalkyl substances [PFAS] and lithium) listed in Table 1. With this latest action, the data released to date represent approximately 46% of the total results that the EPA expects to receive by completion of data reporting in 2026. The agency will update the results quarterly in the UCMR 5 Data Finder and occurrence data text files in addition to updating this Data Summary. Data are added and possibly removed or updated over the course of this reporting cycle following further review by analytical laboratories, public water systems (PWSs), states, and the EPA. Before conducting your own assessment of the data, please review the Data Considerations section. For answers to common questions on accessing and understanding the UCMR 5 data, and on PFAS and lithium in drinking water, please review the UCMR 5 website.

The UCMR 5 dataset:

- Improves the EPA's understanding of the frequency that these contaminants are found in the nation's PWSs, and at what levels.
- Enables a better understanding of where and to what extent different PFAS co-occur with each other in drinking water.
- Helps the agency make determinations about future regulations and other actions to protect public health under the Safe Drinking Water Act (SDWA).
- Assists federal, state, and other researchers in prioritizing studies for health effects information, identifying data gaps, and determining the need for future studies to improve our understanding of the possible health risks associated with these contaminants in public drinking water.

On April 10, 2024, the EPA announced the final National Primary Drinking Water Regulation (NPDWR) for six PFAS; those six are among the 29 PFAS being monitored in UCMR 5. **Relevant information provided in this document is for technical assistance only and does not supersede the NPDWR requirements in 40 CFR 141 and 40 CFR 142**. Starting in April 2029, PWSs (specifically, community and non-transient non-community water systems) will be required to comply with the PFAS NPDWR Maximum Contaminant Levels (MCLs). Therefore, **UCMR 5 results for the regulated PFAS do not indicate compliance or noncompliance with the MCLs**. PWSs may work with their state to submit their UCMR 5 monitoring data to meet some or all of the PFAS NPDWR's initial monitoring requirements, which must be completed by April 2027. For more information on the MCLs and requirements, refer to the EPA's "PFAS NPDWR Monitoring and Reporting" Fact Sheet.

Starting in April 2029, compliance with the PFAS NPDWR MCLs will be determined by calculating the running annual average (RAA) of quarterly results for each sample point, based on compliance monitoring data reported to the primacy agency. With this in mind, and recognizing that the agency only has a partial set of UCMR 5 data, the EPA notes the following:

- For context, the EPA compared UCMR 5 results for the regulated PFAS to their associated MCLs if there are sufficient data available to calculate an annual average for a sampling location. Doing so requires a full set of UCMR 5 results (*i.e.*, two sample results for locations with ground water sources, four sample results for locations with surface water sources).
    - To date, 11% of the PWSs that have reported a full set of UCMR 5 results for at least one location had an average for one or more of the newly regulated PFAS that was greater than the respective MCL(s).

  - Five PFAS have individual MCLs associated with the EPA’s PFAS NPDWR. To date, 9.1%, 7.1%, 0.0%, 0.8%, and 0.1% of PWSs with a full set of UCMR 5 results for at least one location had an average that was greater than the individual MCLs for PFOS, PFOA, HFPO-DA, PFHxS, and PFNA, respectively.
  - Along with PFHxS, PFNA, and HFPO-DA, one additional PFAS (PFBS) is included in the Hazard Index (HI) MCL. To date, 1.0% of PWSs with a full set of UCMR 5 results for at least one location had an average that was greater than the HI MCL.
- Two PFAS (PFBA and PFHxA) have non-regulatory health-based reference concentrations in drinking water (*i.e.*, U.S. Geological Survey [USGS] health-based screening levels [HBSLs] based on the EPA’s Integrated Risk Information System [IRIS] assessments). Neither of these PFAS have been reported above their reference concentrations.
- Non-regulatory health-based reference concentrations in drinking water have not been established for the other (unregulated) 21 PFAS that are part of UCMR 5.
  - Sixteen of these 21 PFAS were measured at or above their respective UCMR minimum reporting level (MRL) in at least one sample by at least one PWS.
  - For the other five PFAS, no PWSs have reported results at or above their respective UCMR MRLs.
- UCMR 5 data show that PFAS co-occur as mixtures in drinking water systems. For example, 65% of sampling locations with at least one PFAS result at or above the UCMR MRL have reported results for multiple PFAS at or above the UCMR MRL(s). The EPA will continue to evaluate the co-occurrence of PFAS in PWSs and at sampling locations as the agency gathers more UCMR 5 monitoring data.
- The EPA established a non-regulatory health-based reference concentration (*i.e.*, EPA’s health reference level [HRL]) for lithium for screening purposes. To date, 25% of PWSs have reported lithium results above the reference concentration.

Regulatory levels (*e.g.*, MCLs), health-based reference values, and other contaminant health effects information is provided in Table 2. Summary details for contaminant occurrence to date, including comparisons to the PFAS NPDWR MCLs and PFAS co-occurrence, are shown in Table 3, Table 4, and Table 5.

Background

The EPA uses the UCMR program to collect nationally representative data for contaminants that may be present in drinking water but are not currently subject to regulatory standards set under SDWA. This monitoring is used by the agency to understand the frequency and level of occurrence of unregulated contaminants in the nation's PWSs. Every five years, taking into consideration the EPA's Contaminant Candidate List (CCL), the agency develops a new list of UCMR contaminants for monitoring. SDWA, as amended by Section 2021 of America's Water Infrastructure Act of 2018, calls for the EPA to:

- Issue a list of unregulated contaminants to be monitored by certain PWS types[1] every five years.
- Require all large PWSs[1] (*i.e.*, those serving more than 10,000 people) to monitor their water for the contaminants.
- Require all small PWSs[1] serving between 3,300 and 10,000 people to monitor, subject to the availability of EPA appropriations and sufficient laboratory capacity.
- Require a nationally representative sample of small PWSs serving fewer than 3,300 people to monitor.
- Pay for the analysis of UCMR samples from participating PWSs serving 10,000 or fewer.
- Make analytical results available in a National Contaminant Occurrence Database (NCOD) for drinking water.

State and local officials may also use the UCMR data to assess the need for actions to protect public health. When evaluating the UCMR data, one should consider the following:

- UCMR monitoring generates a robust dataset that is representative of national occurrence in drinking water.
    - Once data reporting is complete, the UCMR 5 dataset will also be representative of occurrence at the state and local levels for all PWSs[1] serving ≥3,300 people.
- UCMR results are available after PWSs and the laboratories that support their monitoring have reported results to the EPA (up to four months after the samples are collected). Small PWS results may be available sooner relative to large PWS results since the laboratories contracted by the EPA to analyze small PWS samples are contractually obligated to report results within a shorter timeframe.
- There is information about health effects and treatment techniques to address some of these unregulated contaminants.

Through the Bipartisan Infrastructure Law, the EPA is helping states, Tribes, and especially small, rural, and disadvantaged communities to leverage billions of dollars in funding dedicated to investments in infrastructure solutions. Those investments will allow communities to remove emerging contaminants like PFAS from their drinking water. More information about available funding to assist with implementing PFAS testing and treatment at PWSs, including the Bipartisan Infrastructure Law Drinking Water State Revolving Fund Emerging Contaminant supplemental and the Emerging Contaminants in Small or Disadvantaged Communities Grant Program, can be found on the EPA's website. The EPA's free Water Technical Assistance Programs are also available to support communities to develop plans, build technical, managerial, and financial capacity, and access water infrastructure funding.

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[1] UCMR 5 requirements apply to community water systems (CWSs) and non-transient non-community water systems (NTNCWSs). They do not apply to transient non-community water systems (TNCWSs). The use of "PWS" throughout this document refers to CWSs and NTNCWSs participating in UCMR monitoring. For more information on PWS types, visit the agency's website.

Table 1. Contaminants and Methods

Contaminant[1]	CASRN[2]	EPA Method	Contaminant Classification
lithium	7439-93-2	200.7	Metal/Pharmaceutical
perfluorooctanesulfonic acid (PFOS)	1763-23-1	533	PFAS
perfluorooctanoic acid (PFOA)	335-67-1	533	PFAS
hexafluoropropylene oxide dimer acid (HFPO-DA) (GenX chemicals)	13252-13-6	533	PFAS
perfluorohexanesulfonic acid (PFHxS)	355-46-4	533	PFAS
perfluorononanoic acid (PFNA)	375-95-1	533	PFAS
perfluorobutanesulfonic acid (PFBS)	375-73-5	533	PFAS
perfluorobutanoic acid (PFBA)	375-22-4	533	PFAS
perfluorohexanoic acid (PFHxA)	307-24-4	533	PFAS
perfluorodecanoic acid (PFDA)	335-76-2	533	PFAS
11-chloroeicosafluoro-3-oxaundecane-1-sulfonic acid (11Cl-PF3OUdS)	763051-92-9	533	PFAS
1H, 1H, 2H, 2H-perfluorodecane sulfonic acid (8:2 FTS)	39108-34-4	533	PFAS
1H, 1H, 2H, 2H-perfluorohexane sulfonic acid (4:2 FTS)	757124-72-4	533	PFAS
1H, 1H, 2H, 2H-perfluorooctane sulfonic acid (6:2 FTS)	27619-97-2	533	PFAS
4,8-dioxa-3H-perfluorononanoic acid (ADONA)	919005-14-4	533	PFAS
9-chlorohexadecafluoro-3-oxanone-1-sulfonic acid (9Cl-PF3ONS)	756426-58-1	533	PFAS
nonafluoro-3,6-dioxaheptanoic acid (NFDHA)	151772-58-6	533	PFAS
perfluoro (2-ethoxyethane) sulfonic acid (PFEESA)	113507-82-7	533	PFAS
perfluoro-3-methoxypropanoic acid (PFMPA)	377-73-1	533	PFAS
perfluoro-4-methoxybutanoic acid (PFMBA)	863090-89-5	533	PFAS
perfluorododecanoic acid (PFDoA)	307-55-1	533	PFAS
perfluoroheptanesulfonic acid (PFHpS)	375-92-8	533	PFAS
perfluoroheptanoic acid (PFHpA)	375-85-9	533	PFAS
perfluoropentanesulfonic acid (PFPeS)	2706-91-4	533	PFAS
perfluoropentanoic acid (PFPeA)	2706-90-3	533	PFAS
perfluoroundecanoic acid (PFUnA)	2058-94-8	533	PFAS
n-ethyl perfluorooctanesulfonamidoacetic acid (NEtFOSAA)	2991-50-6	537.1	PFAS
n-methyl perfluorooctanesulfonamidoacetic acid (NMeFOSAA)	2355-31-9	537.1	PFAS
perfluorotetradecanoic acid (PFTA)	376-06-7	537.1	PFAS
perfluorotridecanoic acid (PFTrDA)	72629-94-8	537.1	PFAS

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[1] UCMR 5 contaminants are being monitored under the UCMR Assessment Monitoring (AM) design. For more information, refer to the EPA's UCMR 5 website.

[2] CASRN – Chemical Abstracts Service Registry Number

Information About UCMR 5 Results

The purpose of this document is to (1) summarize UCMR 5 results reported to date and (2) provide context around UCMR 5 results in relation to EPA-established UCMR minimum reporting levels (MRLs) and, if available, health-based reference values (*e.g.*, non-regulatory reference concentrations and reference doses [RfDs]) and regulatory values (*e.g.*, MCLs).

The UCMR 5 MRLs are the lowest concentrations that laboratories may report to the EPA during UCMR 5 monitoring. UCMR MRLs are determined using data from multiple laboratories that participate in the EPA's MRL-setting studies and are not associated with contaminant health effects information. The EPA establishes UCMR MRLs to ensure consistency in the quality of the information reported to the agency.

Depending on the available health and toxicological information for a UCMR contaminant, a non-regulatory health-based reference concentration in drinking water may be available. Reference concentrations can be derived from an RfD (*i.e.*, a non-cancer endpoint) or an oral cancer slope factor (CSF) (*i.e.*, a cancer endpoint), if available, and consider additional assumptions about body weight and drinking water intake. Reference concentrations presented in this document do not represent regulatory limits or action levels and should not be interpreted as an indication of future agency actions.

Community water systems (CWSs) required to monitor under UCMR must inform their customers of UCMR results (including the average and range of results) in their annual Consumer Confidence Report (CCR). See 40 CFR 141.153(d)(7) for the CCR regulatory requirements and Section IV of the EPA's guidance Preparing Your Drinking Water Consumer Confidence Report for details on the content of the report. Additional resources are available on the EPA's CCR Compliance Help webpage. Non-transient non-community water systems (NTNCWSs) (*e.g.*, a school that operates its own drinking water system) and CWSs required to monitor under UCMR must inform their customers of the availability of UCMR results through Tier 3 Public Notification (PN). See 40 CFR 141.207 for the PN regulatory requirements and the EPA's PN Compliance Help webpage for guidance. CCR and PN requirements apply to all UCMR results (including results for the six UCMR 5 PFAS that are now subject to the NPDWR) and are separate from the PFAS NPDWR CCR and PN requirements.

The EPA recognizes the high interest in timely access to UCMR results and is committed to publicly posting results on the agency's Occurrence Data webpage approximately quarterly (following large PWS review of their UCMR results and EPA review of small PWS results). The EPA manages the laboratory analyses for small PWSs and will work to communicate their results in a timely manner. Large PWSs wishing to have earlier access to their data should consider making arrangements with their UCMR 5 laboratory for early notification of UCMR results (*i.e.*, before their contracted laboratory posts the results to the UCMR web-based reporting system).

UCMR occurrence data are used to inform the agency's Regulatory Determination process (*i.e.*, the process that addresses potential regulatory actions for unregulated contaminants). States may also establish requirements or levels (regulatory or non-regulatory) for drinking water contaminants. PWSs are responsible for being aware of and complying with their state's requirements, if any.

Available drinking water treatment information for UCMR 5 contaminants can be found in the EPA's Drinking Water Treatability Database. The EPA's PFAS website provides additional information on agency actions to address PFAS contamination, describes current PFAS research, and identifies related tools and resources. The EPA has also published a PFAS Communication Toolkit to help PWSs and community leaders educate the public about PFAS, where they come from, their health risks, how to reduce exposure, and about the final PFAS NPDWR.

Health-Based Reference Values

Table 2 provides health-based reference values (*i.e.*, non-regulatory health-based reference concentrations and RfDs) for each contaminant monitored under UCMR 5, if available. To identify reference values, the EPA applied the following principles:

(1) Reference concentrations and RfDs were compiled from the following publicly available resources:
   a. EPA Technical Support Document for the Final CCL 5 – Contaminant Information Sheets and
   b. EPA Integrated Risk Information System (IRIS) Assessments
   c. U.S. Geological Survey (USGS) Health-Based Screening Levels (HBSLs)

   The above resources are the products (or compilation) of peer-reviewed health assessments. The reference values are subject to change as new health assessments are completed; they are not legally enforceable federal standards.

(2) If health information was available from more than one of the resources listed above, the most recent health information was used.

(3) If both cancer and non-cancer reference concentrations were available from the most recent resource, the lower of the two concentrations was used. Please review the references and footnotes in Table 2 for additional health effects information.

(4) If an RfD (*i.e.*, a non-cancer endpoint) was the basis for the reference concentration, and both chronic and subchronic/short-term exposure values were available from the most recent resource, the lower concentration (associated with the chronic exposure) was used. Please review the references and footnotes in Table 2 for additional health effects information (*e.g.*, additional short-term, subchronic, or chronic values).

(5) For the contaminants that do not have a reference concentration available from a resource listed above, only the RfDs from finalized health assessments are provided in Table 2, if available. If a health assessment is in process, a link to additional information about its status is provided.

The EPA considers this a "living document" and will update Table 2 as new health-based information becomes available.

Table 2. UCMR Minimum Reporting Levels (MRLs), Regulatory Levels, and Health-Based Reference Values

Contaminant [Note: to convert to ng/L or parts per trillion (ppt), multiply by 1,000]	UCMR MRL (µg/L)[1]	Regulatory Level (µg/L)	Health-Based Reference Values		References
			Non-Regulatory Reference Concentration (µg/L)	RfD (mg/kg-day)	
lithium	9	-	HRL[2] = 10	subchronic and chronic provisional RfD = 2×10^{-3}	Technical Support Document for the Final CCL 5 - Contaminant Information Sheets
PFOS	0.004	MCL[3] = 0.0040	-	-	2024 Final PFAS NPDWR
PFOA	0.004	MCL[3] = 0.0040	-	-	2024 Final PFAS NPDWR
HFPO-DA (GenX chemicals)	0.005	MCL[3] = 0.01	-	-	2024 Final PFAS NPDWR
PFHxS[4]	0.003	MCL[3] = 0.01	-	-	2024 Final PFAS NPDWR
PFNA[4]	0.004	MCL[3] = 0.01	-	-	2024 Final PFAS NPDWR
PFBS[5]	0.003	-	-	-	2024 Final PFAS NPDWR
PFBA	0.005	-	HBSL[6] = 6	chronic RfD = 1×10^{-3} subchronic RfD = 6×10^{-3}	2024 USGS Health-Based Screening Level
PFHxA	0.003	-	HBSL[6] = 3	subchronic and chronic RfD = 5×10^{-4}	2024 USGS Health-Based Screening Level
PFDA	0.003	-	-	-	In process/Draft IRIS Assessment
11Cl-PF3OudS	0.005	-	-	-	-
8:2 FTS	0.005	-	-	-	-
4:2 FTS	0.003	-	-	-	-
6:2 FTS	0.005	-	-	-	-

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[1] UCMR MRL – EPA-established UCMR Minimum Reporting Level. Based on laboratory capability; not related to contaminant health effects information.

[2] HRL – Health Reference Level calculated as part of the CCL 5 process. See Terms and Definitions. The HRL for lithium is based on the RfD from the following health assessment: Provisional Peer-Reviewed Toxicity Values for Lithium (2008). For more information, see the EPA's Technical Fact Sheet on Lithium in Drinking Water for primacy agencies.

[3] MCL – Maximum Contaminant Level. See Terms and Definitions and the PFAS NPDWR section of this document.

[4] In process/draft EPA Integrated Risk Information System (IRIS) assessments for PFHxS and PFNA.

[5] PFBS has a Health-Based Water Concentration (HBWC) of 2 µg/L associated with the final PFAS NPDWR. PFBS is not regulated individually; it is included in the Hazard Index (HI) calculation when PFBS occurs in a mixture with one or more of HFPO-DA, PFHxS, and PFNA. See Terms and Definitions and the PFAS NPDWR section of this document.

[6] HBSL – USGS Health-Based Screening Level. See Terms and Definitions. The HBSLs are based on the RfDs from the EPA's IRIS Assessments for PFBA and PFHxA.

Contaminant [Note: to convert to ng/L or parts per trillion (ppt), multiply by 1,000]	UCMR MRL (µg/L)[1]	Regulatory Level (µg/L)	Health-Based Reference Values		References
			Non-Regulatory Reference Concentration (µg/L)	RfD (mg/kg-day)	
ADONA	0.003	-	-	-	-
9Cl-PF3ONS	0.002	-	-	-	-
NFDHA	0.02	-	-	-	-
PFEESA	0.003	-	-	-	-
PFMPA	0.004	-	-	-	-
PFMBA	0.003	-	-	-	-
PFDoA	0.003	-	-	-	-
PFHpS	0.003	-	-	-	-
PFHpA	0.003	-	-	-	-
PFPeS	0.004	-	-	-	-
PFPeA	0.003	-	-	-	-
PFUnA	0.002	-	-	-	-
NEtFOSAA	0.005	-	-	-	-
NMeFOSAA	0.006	-	-	-	-
PFTA	0.008	-	-	-	-
PFTrDA	0.007	-	-	-	-

Table 3. July 2024 UCMR 5 Data Summary for Unregulated Contaminants[1]

Contaminant	UCMR MRL[2] (µg/L)	Ref Conc[3] (µg/L)	Total number of results	Number of results ≥MRL	Number of results >Ref Conc[4]	% of total results >Ref Conc	Total number of PWSs with results	Number of PWSs with results ≥MRL	Number of PWSs with results >Ref Conc[4]	% of PWSs with results >Ref Conc
lithium	9	10	32,343	9,104	6,338	19.6%	6,520	2,248	1,626	24.9%
PFBA	0.005	6	31,487	2,653	0	0.0%	6,401	1,101	0	0.0%
PFHxA	0.003	3	31,496	2,981	0	0.0%	6,403	1,040	0	0.0%
PFDA	0.003	-	31,508	16	-	-	6,403	6	-	-
11Cl-PF3OUdS	0.005	-	31,508	0	-	-	6,402	0	-	-
8:2 FTS	0.005	-	31,501	5	-	-	6,402	5	-	-
4:2 FTS	0.003	-	31,506	2	-	-	6,402	2	-	-
6:2 FTS	0.005	-	31,493	156	-	-	6,402	111	-	-
ADONA	0.003	-	31,507	3	-	-	6,402	2	-	-
9Cl-PF3ONS	0.002	-	31,486	1	-	-	6,402	1	-	-
NFDHA	0.02	-	31,500	4	-	-	6,402	3	-	-
PFEESA	0.003	-	31,508	0	-	-	6,403	0	-	-
PFMPA	0.004	-	31,507	3	-	-	6,403	2	-	-
PFMBA	0.003	-	31,507	2	-	-	6,403	1	-	-
PFDoA	0.003	-	31,501	2	-	-	6,403	2	-	-
PFHpS	0.003	-	31,507	2	-	-	6,403	2	-	-
PFHpA	0.003	-	31,504	751	-	-	6,403	311	-	-
PFPeS	0.004	-	31,503	64	-	-	6,403	34	-	-
PFPeA	0.003	-	31,483	3,376	-	-	6,403	1,148	-	-
PFUnA	0.002	-	31,500	3	-	-	6,403	2	-	-
NEtFOSAA	0.005	-	32,109	1	-	-	6,490	1	-	-
NMeFOSAA	0.006	-	32,109	0	-	-	6,490	0	-	-
PFTA	0.008	-	32,109	0	-	-	6,490	0	-	-
PFTrDA	0.007	-	32,108	0	-	-	6,490	0	-	-

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[1] This data summary represents approximately 46% of total results that the EPA expects to receive by completion of data reporting in 2026. Analytical results from the UCMR program are reported by laboratories and provided by the agency in micrograms/liter (µg/L, or parts per billion). To convert results in µg/L to nanograms/liter (ng/L, or parts per trillion), multiply the value by 1,000. The UCMR results represented by this table are single measurements and do not represent a running annual average (RAA). For information on results to date for the regulated PFAS, see the PFAS NPDWR section of this document. The total number of results and total number of PWSs with results for the regulated PFAS are similar to the other EPA Method 533 PFAS (*i.e.*, approximately 31,500 results from more than 6,400 PWSs).

[2] UCMR MRL – EPA-established UCMR Minimum Reporting Level. Based on laboratory capability; not related to contaminant health effects information.

[3] Ref Conc – Reference Concentration. Based on contaminant health effects information; non-regulatory and non-enforceable. The EPA's CCL 5 Health Reference Level (HRL) for lithium and the USGS Health-Based Screening Levels (HBSLs) for PFBA and PFHxA. See Terms and Definitions.

[4] The HRL and the HBSLs are expressed with one significant digit; comparison of UCMR results to those levels is therefore based on one significant digit. Results >15 µg/L for lithium round to 20 µg/L; results >6.5 µg/L for PFBA round to 7 µg/L; and results >3.5 µg/L for PFHxA round to 4 µg/L and are identified as above the reference concentrations.

Final PFAS NPDWR

In April 2024, the EPA established legally enforceable standards for five individual PFAS: PFOA, PFOS, PFNA, PFHxS, and HFPO-DA (known as GenX chemicals). The agency's regulatory determination for PFNA, PFHxS, and HFPO-DA is based on their substantial likelihood to occur in PWSs with a frequency and at levels of health concern. The EPA also established an enforceable standard for mixtures containing two or more of PFNA, PFHxS, HFPO-DA, and PFBS. Please refer to the PFAS NPDWR website for more information. **UCMR 5 results for the regulated PFAS do not indicate current compliance or noncompliance with the MCLs.** Compliance with the PFAS regulatory MCLs will be determined by calculating the running annual average (RAA) of quarterly results for each sample point based on compliance monitoring data reported to the primacy agency.

The EPA currently has a partial UCMR 5 dataset, with approximately 3,500 PWSs reporting full sets of results (*i.e.*, two results for locations with ground water sources and four results for locations with surface water sources) for approximately 8,900 sampling locations. Recognizing that the UCMR 5 results have no direct implications for PWS MCL compliance, but that many are interested in comparing UCMR 5 data to the MCLs, the EPA calculated annual averages for the UCMR 5 results where such a calculation was possible. The agency then compared those averages to the NPDWR MCLs. Table 4 presents the UCMR 5 results to date using sampling location averages and the MCLs from the PFAS NPDWR. Approximately 11% of the PWSs in this group had an average greater than an individual MCL for at least one regulated PFAS and/or for the HI MCL at one or more sampling locations. Please note: if a particular PWS had averages greater than multiple MCLs, that PWS will be counted in this table multiple times (*i.e.*, once in each row for the respective PFAS with an average greater than the MCL). If this is not considered by those assessing the data in these rows, it would result in "double counting." For more information on calculating averages for the PFAS MCLs, please refer to Section VIII of the final PFAS NPDWR *Federal Register* notice, 40 CFR 141.903, and the PFAS NPDWR website.

Table 4. July 2024 Comparison of UCMR 5 Average Results and the MCLs for Regulated PFAS

Regulated PFAS	MCL (µg/L)[1]	Total number of locations with a full set of results[2]	Number of locations with an average greater than MCL	% of locations with an average greater than MCL	Total number of PWSs with location(s) with a full set of results	Number of PWSs with average(s) greater than MCL	% of PWSs with average(s) greater than MCL
PFOS	0.0040	8,887	524	5.9%	3,459	316	9.1%
PFOA	0.0040	8,888	445	5.0%	3,460	246	7.1%
HFPO-DA (GenX chemicals)	0.01	8,893	1	0.0%	3,462	1	0.0%
PFHxS	0.01	8,888	38	0.4%	3,460	29	0.8%
PFNA	0.01	8.892	3	0.0%	3,462	3	0.1%
Hazard Index (HFPO-DA, PFHxS, PFNA, PFBS)	1 (unitless)	8,880	41	0.5%	3,455	33	1.0%
Total number of unique PWSs with one or more averages greater than MCL = 393 of 3,463 (11%)							

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[1] MCLs for PFOA and PFOS are expressed with two significant digits; MCLs for HFPO-DA, PFHxS, PFNA, and the HI are expressed with one significant digit. Comparison of UCMR 5 averages to MCLs is based on the corresponding number of significant digits. An average is counted as greater than the MCL for PFOS or PFOA if it is ≥0.00405 µg/L. An average is counted as greater than the MCL for HFPO-DA, PFHxS, or PFNA if it is ≥0.015 µg/L. An average is counted as greater than the HI MCL if it is ≥1.5 and at least two PFAS included in the average are measured at or above the UCMR MRL.

[2] For UCMR 5 monitoring, PWSs may have multiple sampling locations, for which there are either two or four sample events over a period of 12 months (for locations with ground water or surface water sources, respectively). Sampling locations were only considered in the comparison to each MCL if they had a corresponding full set of UCMR 5 results (*i.e.*, two or four results). Note: compliance with the PFAS NPDWR MCLs will be determined by calculating the running annual average of four quarterly results for each sample point. When calculating annual averages using UCMR 5 results for comparison with the MCLs, the average for locations with ground water sources is based on two semi-annual results and the average for locations with surface water sources is based on four quarterly results.

UCMR 5 PFAS Co-occurrence in Drinking Water

The EPA's examination of drinking water data shows that different PFAS can often be found together and in varying combinations as mixtures (for additional discussion, please see the EPA's PFAS Occurrence and Contaminant Background Support Document). Additionally, decades of research show mixtures of different chemicals can have additive health effects, even if the individual chemicals are each present at lower levels. The EPA has established drinking water standards for certain PFAS to provide health protection against these individual and co-occurring PFAS in PWSs. In cases where the PFAS included in the final PFAS NPDWR occur at concentrations above their respective regulatory standards, there is also an increased probability of co-occurrence of additional unregulated PFAS. As discussed in the final PFAS NPDWR, the EPA expects that compliance actions taken under the final rule will remove unregulated co-occurring PFAS contaminants and provide additional public health protection and benefits because the best available drinking water treatment technologies have been demonstrated to co-remove other PFAS and non-PFAS contaminants that may have adverse health effects.

Table 5 provides a general assessment of UCMR 5 PFAS co-occurrence by location (*i.e.*, considering all available PFAS results to date for a sampling location). For UCMR 5 monitoring, PWSs may have multiple sampling locations. Each sample event includes sample collection for 29 PFAS. This table presents the count of sampling locations for which "N or more" unique PFAS were found at or above the UCMR MRL, where N is 1-11 in Table 5. The table stops at 11 (and not 29) because 11 was the maximum number of unique PFAS found to co-occur at a sampling location (*i.e.*, same PWS, facility, and sample point). Results were included in the location-level counts regardless of whether results were available for all 29 PFAS for a sampling location.

Table 5. July 2024 UCMR 5 PFAS Co-occurrence Counts by Sampling Location

Number (N) of Unique PFAS ≥UCMR MRL[1]	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
Number of Sampling Locations with N or More PFAS[2]	3,736	2,434	1,824	1,334	934	599	371	185	56	11	4
Number of Unique PWSs Associated with Locations[3]	*2,848*	*1,875*	*1,416*	*1,039*	*719*	*455*	*277*	*142*	*45*	*11*	*4*

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[1] Represents the number (N) "or more" count of unique PFAS found at or above their UCMR Minimum Reporting Level (MRL). UCMR MRLs are based on laboratory capability and are not related to contaminant health effects information.

[2] Represents the number of individual sampling locations with the corresponding number of unique PFAS found across all available results to date for the location. For example, 1,824 sampling locations each had three or more different PFAS occur; these 1,824 sampling locations are from 1,416 unique PWSs.

[3] Represents the number of unique PWSs associated with the number of sampling locations for each count. For example, 1,416 different PWSs each had at least one sampling location with three or more different PFAS occur.

Terms and Definitions

a) **HBSL** – USGS non-cancer Health-Based Screening Level. HBSLs are non-enforceable water quality benchmark concentrations of contaminants in water developed using the latest EPA methods for establishing drinking water guidelines and the most recent EPA peer-reviewed toxicity information. Non-cancer HBSLs are maximum concentrations that are not expected to cause adverse non-carcinogenic health effects over a lifetime of exposure.

b) **HBWC** – Health-Based Water Concentration. The level below which there are no known or anticipated adverse health effects over a lifetime of exposure, including sensitive populations and life stages, and allows for an adequate margin of safety.

c) **HI** – Hazard Index. A long-established approach that the EPA regularly uses to understand health risk from a chemical mixture (*i.e.*, exposure to multiple chemicals). The HI is made up of a sum of fractions. Each fraction compares the level of each PFAS measured in the water to the HBWC. The HI is the sum of component hazard quotients, which are calculated by dividing the measured PFAS component contaminant concentration in water [*e.g.*, expressed as parts per trillion (ppt) or nanograms per liter (ng/L)] by the associated HBWC expressed in the same units as the measured concentration (*e.g.*, ppt or ng/L). For PFAS, a mixture HI greater than 1 (unitless) is an exceedance of the HI MCL.

d) **HRL** – Health Reference Level. Derived during the EPA's Contaminant Candidate List (CCL) process for screening purposes. HRLs are used in the EPA's Regulatory Determination process as risk-derived concentrations against which to evaluate occurrence data to determine if contaminants occur at levels of public health concern. HRLs are not final determinations about the level of a contaminant in drinking water that is necessary to protect any particular population and, in some cases, are derived prior to development of a complete exposure assessment using the best available data. HRLs are not legally enforceable federal standards. To determine the HRL for a chemical, the agency considers adverse health effects that may pose a greater risk to specific life stages and other sensitive groups which represent a meaningful portion of the population. For more information on HRL derivation, please see the Technical Support Document for the Final CCL 5 – Contaminant Information Sheets.

e) **MCL** – Maximum Contaminant Level. The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards.

f) **MCLG** – Maximum Contaminant Level Goal. The level of a contaminant in drinking water at which there is no known or expected risk to health. MCLGs allow for a margin of safety and are non-enforceable public health goals.

g) **Ref Conc** – Reference Concentration. Based on publicly available health information found in the following resources: EPA CCL 5 Contaminant Information Sheets [*i.e.*, Health Reference Levels (HRLs)], USGS Health-Based Screening Levels (HBSLs). Reference concentrations are derived from peer-reviewed health assessments published by the EPA or other governmental agencies. They are not legally enforceable federal standards and are subject to change as new health assessments are completed. Depending on available health effects information, a reference concentration in drinking water can be derived from a reference dose (RfD) (*i.e.*, a non-cancer endpoint) or a cancer slope factor (CSF) (*i.e.*, a cancer endpoint), and considers additional assumptions about body weight and drinking water intake.

h) **RfD** – Oral Reference Dose. A non-cancer estimate (with uncertainty spanning perhaps an order of magnitude) of a daily oral exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It is typically derived by dividing a point-of-departure (POD) from a selected dose-response study (*e.g.*, no-observed-adverse-effect level [NOAEL], lowest-observed-adverse-effect level [LOAEL], benchmark dose [BMD]) by the uncertainty factors (UFs) applied to reflect limitations of the data used. Chronic RfDs are typically derived from animal toxicological studies with an exposure duration of months to years, representing a lifetime exposure in humans. Subchronic RfDs are typically derived from animal toxicological studies with an exposure duration of 31 to 90 days, representing a less than lifetime exposure in humans (up to 10% of average lifespan). Visit the EPA's IRIS website for more information about RfD derivation.

i) **UCMR MRL** – EPA-established UCMR Minimum Reporting Level. The lowest concentration that laboratories may report to the EPA during UCMR 5 monitoring. MRLs are not associated with health effects information. More specifically, an MRL is the quantitation limit for a contaminant that is considered achievable, with 95% confidence, by at least 75% of laboratories nationwide using a specified analytical method (recognizing that individual laboratories may be able to measure at lower levels). **[Note: The Agency for Toxic Substances and Disease Registry (ATSDR) uses the term "MRL" for a different purpose (*i.e.*, to describe "Minimal Risk Level"). The UCMR term and the ATSDR term have no relationship to each other.]**

Data Considerations

The UCMR 5 analytical results are publicly available through the UCMR 5 Data Finder and as text files.

The UCMR 5 Data Finder allows people to easily search for, summarize, and download the available UCMR 5 analytical results. Results can be filtered using multiple data fields, including PWS, PWS size, state, EPA Region, contaminant, source water type, results at or above UCMR MRLs, and results above health-based reference concentrations (data definitions provided in Table 6). The UCMR 5 Data Finder can be used by federal, state, and local agencies as well as the public to easily locate and retrieve specific results and assist with answering questions regarding UCMR 5 monitoring. Selected results can be viewed online or downloaded as a Microsoft Excel file (.xlsx). A video demonstration of the UCMR 5 Data Finder is available here.

For those interested in large-scale data processing using statistical or data analysis software, the EPA recommends using the occurrence data text files containing the UCMR 5 analytical results as well as additional information reporting during monitoring. Data are provided in tab delimited text files (.txt) (see below for descriptions), with field names included in the first row of each file and no text qualifier. The EPA recommends importing all ID fields into your choice of software as text since some of the IDs can otherwise be misinterpreted as long integer field types when they contain alpha characters.

- To download the occurrence data text files (data definitions provided in Table 7), select one of the following zip (.zip) files from UCMR 5 (2023-2025) Occurrence Data:
    - **UCMR 5 Occurrence Data Text Files** to view all the analytical results to date (*i.e.*, results for all contaminants reported by all PWSs). The **UCMR5_All.txt** file will likely become too large to be imported into Excel once the majority of the UCMR 5 results are reported, in which case you can try other applications (*e.g.*, Microsoft Access) or import a subset of the data as described below.
    - **UCMR 5 Occurrence Data Text Files by State** to view all the analytical results to date, organized by Tribes and states. Within that zip file, one text file (**UCMR5_All_Tribes_AK_LA.txt**) will have all results for Tribal PWSs and for the states starting alphabetically with A through L; another file (**UCMR5_All_MA_WY.txt**) will have all results for the states starting alphabetically with M through W. The results are organized this way to address file size limitations and streamline data management.
    - **UCMR 5 Occurrence Data Text Files by Method Classification** to view all the analytical results to date, organized by analytical method. Within that zip file, you will find individual text files with results organized by method (*e.g.*, a Method 200.7 file with results for lithium).
- The following text files for **additional data elements** (*i.e.*, information beyond analytical results for the 30 UCMR 5 contaminants) are also contained in each of the above zip files:
    - **UCMR5_ZIPCodes.txt** – U.S. Postal Service ZIP Code(s) for all areas served by a PWS (data definitions provided in Table 8)
    - **UCMR5_AddtlDataElem.txt** – Disinfectant Type, Treatment Information, Lithium Occurrence, Lithium Treatment, PFAS Occurrence, PFAS Treatment, Potential PFAS Sources, Potential PFAS Sources Detail (data definitions provided in Table 9)
        - The EPA is not asking PWSs for a formal, in-depth, source water evaluation for potential PFAS sources and recognizes that some PWSs will have more complete information than others. The agency's PFAS Analytic Tools can serve as a starting point to answer this question and are accessible here. UCMR 5 data will be updated in the PFAS Analytic Tools soon after each quarterly data release.

For step-by-step details on using the UCMR 5 Data Finder and occurrence data text files, please refer to the document Instructions for Accessing UCMR Results. Additional reference material, including common questions and answers on accessing and understanding the UCMR 5 data, is available on the UCMR 5 website.

Table 6. Data Definitions for the UCMR 5 Data Finder

Field Name	Definition
PWS ID	Public Water System (PWS) Identification Code. The code used to identify each PWS. The code begins with the standard 2-character postal state abbreviation or Region code for Tribes; the remaining 7 numbers are unique to each PWS in the state. Utah PWS IDs begin with 4 letters (UTAH) followed by 5 numbers
PWS Name	Name of the PWS
Contaminant	The UCMR 5 contaminant analyzed
Result (µg/L)	Numeric value of the analytical result in µg/L for the contaminant. Results less than the UCMR MRL are indicated by **<MRL**
Health-Based Ref Conc (µg/L)	Non-regulatory Health-Based Reference Concentration in µg/L for the contaminant, if available (see Terms and Definitions)
Collection Date	Date of sample collection (month, day, year)
Facility ID	Identification code for each applicable facility associated with water treatment or delivery at the PWS
Facility Name	Name of the facility at the PWS
Sample Point ID	Identification code for each sample point location at the PWS
Sample Point Name	Name of the sample point at the PWS
Sample Event Code	Identification code for each sample event**:** **SE1**, **SE2**, **SE3**, **SE4**
Sample ID	Identification code for each sample
Method ID	Identification code of the analytical method
PWS Size	Size category of the PWS for UCMR 5, based on retail population as indicated by the Safe Drinking Water Information System (Federal) (SDWIS/FED) as of February 1, 2021: **S** (≤ 10,000), **L** (> 10,000)
Facility Water Type	Source of water at the facility: **SW** (surface water), **GW** (ground water), **GU** (ground water under the direct influence of surface water), **MX** (any combination of SW, GW, and GU)
Sample Point Type	Sampling Point Type Code: **EP** (entry point to the distribution system)
EPA Region	EPA Region (states): **Region 1** (CT, ME, MA, NH, RI, VT), **Region 2** (NJ, NY, PR [Puerto Rico], VI [Virgin Islands]), **Region 3** (DE, DC, MD, PA, VA, WV), **Region 4** (AL, FL, GA, KY, MS, NC, SC, TN), **Region 5** (IL, IN, MI, MN, OH, WI), **Region 6** (AR, LA, NM, OK, TX), **Region 7** (IA, KS, MO, NE), **Region 8** (CO, MT, ND, SD, UT, WY), **Region 9** (AZ, CA, HI, NV, AS [American Samoa], GU [Guam], MP [Northern Marianas Islands], NN [Navajo Nation]), **Region 10** (AK, ID, OR, WA)
State	State abbreviation. Tribal PWSs without primacy are attributed to an EPA Region (01, 02, 03, 04, 05, 06, 07, 08, 09, 10)
UCMR Minimum Reporting Level (MRL, µg/L)	Minimum Reporting Level defined by UCMR 5 in µg/L for the contaminant. Based on laboratory capability; not related to contaminant health effects information (see Terms and Definitions)

Table 7. Data Definitions for Text Files: UCMR5_All, UCMR5_All_Tribes_AK_LA, UCMR5_All_MA_WY, and UCMR5_*MethodNumber*

Field Name	Definition
PWSID	Public Water System (PWS) Identification Code. The code used to identify each PWS. The code begins with the standard 2-character postal state abbreviation or Region code for Tribes; the remaining 7 numbers are unique to each PWS in the state. Utah PWS IDs begin with 4 letters (UTAH) followed by 5 numbers
PWSName	Name of the PWS
Size	Size category of the PWS for UCMR 5, based on retail population as indicated by the Safe Drinking Water Information System (Federal) (SDWIS/FED) as of February 1, 2021: **S** (≤ 10,000), **L** (> 10,000)
FacilityID	Identification code for each applicable facility associated with water treatment or delivery at the PWS
FacilityName	Name of the facility at the PWS
FacilityWaterType	Source of water at the facility: **SW** (surface water), **GW** (ground water), **GU** (ground water under the direct influence of surface water), **MX** (any combination of SW, GW, and GU)
SamplePointID	Identification code for each sample point location at the PWS
SamplePointName	Name of the sample point at the PWS
SamplePointType	Sampling Point Type Code: **EP** (entry point to the distribution system)
AssociatedFacilityID	Null for UCMR 5
AssociatedSamplePointID	Null for UCMR 5
CollectionDate	Date of sample collection (month, day, year)
SampleID	Identification code for each sample
Contaminant	The UCMR 5 contaminant analyzed
MRL	Minimum Reporting Level (MRL) defined by UCMR 5 in µg/L for the contaminant. Based on laboratory capability; not related to contaminant health effects information (see Terms and Definitions)
Units	Units of the UCMR MRL and analytical results: **µg/L**
MethodID	Identification code of the analytical method
AnalyticalResultsSign	Sign indicating whether the analytical result is less than (**<**) the UCMR MRL or equal to (**=**) a numeric value at or above the UCMR MRL
AnalyticalResultValue	Numeric value of the analytical result in µg/L for the contaminants. Null (or blank) values represent results less than the UCMR MRL
SampleEventCode	Identification code for each sample event: **SE1**, **SE2**, **SE3**, **SE4**
MonitoringRequirement	**AM** (Assessment Monitoring)
Region	EPA Region (states): **1** (CT, ME, MA, NH, RI, VT), **2** (NJ, NY, PR [Puerto Rico], VI [Virgin Islands]), **3** (DE, DC, MD, PA, VA, WV), **4** (AL, FL, GA, KY, MS, NC, SC, TN), **5** (IL, IN, MI, MN, OH, WI), **6** (AR, LA, NM, OK, TX), **7** (IA, KS, MO, NE), **8** (CO, MT, ND, SD, UT, WY), **9** (AZ, CA, HI, NV, AS [American Samoa], GU [Guam], MP [Northern Marianas Islands], NN [Navajo Nation]), **10** (AK, ID, OR, WA)
State	State abbreviation. Tribal PWSs without primacy are attributed to an EPA Region (01, 02, 03, 04, 05, 06, 07, 08, 09, 10)
UCMR1SampleType	Null for UCMR 5

Table 8. Data Definitions for Text File: UCMR5_ZIPCodes

Field Name	Definition
ZIPCODE	U.S. Postal Service ZIP Code(s) for all areas served by a PWS. This is entered by the PWS

Table 9. Data Definitions for Text File: UCMR5_AddtlDataElem

Additional Data Element	Definition and Response Options
DisinfectantType	All of the disinfectants/oxidants that have been added prior to and at the entry point to the distribution system. Please select ALL that apply. **PEMB** = permanganate, **HPXB** = hydrogen peroxide, **CLGA** = gaseous chlorine, **CLOF** = offsite generated hypochlorite (stored as a liquid form), **CLON** = onsite generated hypochlorite, **CAGC** = chloramine (formed with gaseous chlorine), **CAOF** = chloramine (formed with offsite hypochlorite), **CAON** = chloramine (formed with onsite hypochlorite), **CLDB** = chlorine dioxide, **OZON** = ozone, **ULVL** = ultraviolet light, **OTHD** = other types of disinfectant/oxidant, **NODU** = no disinfectant/oxidant used
TreatmentInformation	Treatment information associated with the sample point. Please select ALL that apply. **CON** = conventional (non-softening, consisting of at least coagulation/sedimentation basins and filtration), **SFN** = softening, **RBF** = river bank filtration, **PSD** = pre-sedimentation, **INF** = in-line filtration, **DFL** = direct filtration, **SSF** = slow sand filtration, **BIO** = biological filtration (operated with an intention of maintaining biological activity within filter), **UTR** = unfiltered treatment for surface water source, **GWD** = ground water system with disinfection only, **PAC** = application of powder activated carbon, **GAC** = granular activated carbon adsorption (not part of filters in CON, SFN, INF, DFL, or SSF), **AIR** = air stripping (packed towers, diffused gas contactors), **POB** = pre-oxidation with chlorine (applied before coagulation for CON or SFN plants or before filtration for other filtration plants), **MFL** = membrane filtration, **IEX** = ionic exchange, **DAF** = dissolved air floatation, **CWL** = clear well/finished water storage without aeration, **CWA** = clear well/finished water storage with aeration, **ADS** = aeration in distribution system (localized treatment), **OTH** = other types of treatment, **NTU** = no treatment used, **DKN** = do not know
LithiumOccurrence	A yes or no answer provided by the PWS for each entry point to the distribution system. Question: Have you tested for the contaminant in your drinking water in the past? **YES** = If yes, did you modify your treatment and if so, what types of treatment did you implement? (see **LithiumTreatment**); **NO** = have never tested for the contaminant; **DK** = do not know
LithiumTreatment	If yes, select ALL that apply: **PAC** = application of powder activated carbon, **GAC** = granular activated carbon adsorption (not part of filters in CON, SFN, INF, DFL, or SSF), **IEX** = ionic exchange, **NRO** = nanofiltration and reverse osmosis, **OZN** = ozone, **BAC** = biologically active carbon, **MFL** = membrane filtration, **UVL** = ultraviolet light, **OTH** = other, **NMT** = not modified after testing
PFASOccurrence	A yes or no answer provided by the PWS for each entry point to the distribution system. Question: Have you tested for the contaminant in your drinking water in the past? **YES** = If yes, did you modify your treatment and if so, what types of treatment did you implement? (see **PFASTreatment**); **NO** = have never tested for the contaminant; **DK** = do not know
PFASTreatment	If yes, select ALL that apply: **PAC** = application of powder activated carbon, **GAC** = granular activated carbon adsorption (not part of filters in CON, SFN, INF, DFL, or SSF), **IEX** = ionic exchange, **NRO** = nanofiltration and reverse osmosis, **OZN** = ozone, **BAC** = biologically active carbon, **MFL** = membrane filtration, **UVL** = ultraviolet light, **OTH** = other, **NMT** = not modified after testing
PotentialPFASSources	A yes or no answer provided by the PWS for each entry point to the distribution system. Question: Are you aware of any potential current and/or historical sources of PFAS that may have impacted the drinking water sources at your water system? **YES** = If yes, select ALL that apply (see **PotentialPFASSourcesDetail**); **NO** = not aware of any potential current and/or historical sources; **DK** = do not know
PotentialPFASSourcesDetail	If yes, select ALL that apply: **MB** = military base, **FT** = firefighting training school, **AO** = airport operations, **CW** = car wash or industrial launderers, **PS** = public safety activities (*e.g.,* fire and rescue services), **WM** = waste management, **HW** = hazardous waste collection, treatment, and disposal, **UW** = underground injection well, **SC** = solid waste collection, combustors, incinerators, **MF** = manufacturing, **FP** = food packaging, **TA** = textile and apparel (*e.g.,* stain- and water-resistant, fiber/thread, carpet, house furnishings, leather), **PP** = paper, **CC** = chemical, **PR** = plastics and rubber products, **MM** = machinery, **CE** = computer and electronic products, **FM** = fabricated metal products (*e.g.*, nonstick cookware), **PC** = petroleum and coal products, **FF** = furniture, **OG** = oil and gas production, **UT** = utilities (*e.g.,* sewage treatment facilities), **CT** = construction (*e.g.,* wood floor finishing, electrostatic painting), **OT** = other

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Full length article

Per- and polyfluoroalkyl substances (PFAS) in United States tapwater: Comparison of underserved private-well and public-supply exposures and associated health implications

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ABSTRACT

Drinking-water quality is a rising concern in the United States (US), emphasizing the need to broadly assess exposures and potential health effects at the point-of-use. Drinking-water exposures to per- and poly-fluoroalkyl substances (PFAS) are a national concern, however, there is limited information on PFAS in residential tapwater at the point-of-use, especially from private-wells. We conducted a national reconnaissance to compare human PFAS exposures in unregulated private-well and regulated public-supply tapwater. Tapwater from 716 locations (269 private-wells; 447 public supply) across the US was collected during 2016–2021 including three locations where temporal sampling was conducted. Concentrations of PFAS were assessed by three laboratories and compared with land-use and potential-source metrics to explore drivers of contamination. The number of individual PFAS observed ranged from 1 to 9 (median: 2) with corresponding cumulative concentrations (sum of detected PFAS) ranging from 0.348 to 346 ng/L. Seventeen PFAS were observed at least once with PFBS, PFHxS and PFOA observed most frequently in approximately 15% of the samples. Across the US, PFAS profiles and estimated median cumulative concentrations were similar among private wells and public-supply tapwater. We estimate that at least one PFAS could be detected in about 45% of US drinking-water samples. These detection probabilities varied spatially with limited temporal variation in concentrations/numbers of PFAS detected. Benchmark screening approaches indicated potential human exposure risk was dominated by PFOA and PFOS, when detected. Potential source and land-use information was related to cumulative PFAS concentrations, and the number of PFAS detected; however, corresponding relations with specific PFAS were limited likely due to low detection frequencies and higher detection limits. Information generated supports the need for further assessments of cumulative health risks of PFAS as a class and in combination with other co-occurring contaminants, particularly in unmonitored private-wells where information is limited or not available.

1. Introduction

The quality and sustainability of drinking-water are rising concerns in the United States (US) because of population-driven water demands, increasing contamination of drinking-water resources, and a growing understanding of potential human-health consequences associated with

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exposures to contaminants. Per- and poly-fluoroalkyl substances (PFAS), "forever chemicals," are a class consisting of thousands of substances (Glüge et al., 2020) that are national/global human-health concerns due to environmental prevalence and persistence, toxicity, and human exposures through water and food (Evich et al., 2022; Sunderland et al., 2019; Tokranov et al., 2021). Legacy long-chain perfluoroalkyl acids (PFAAs) include perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS), which are historically two of the most widely used and studied chemicals in the PFAS group (Tokranov et al., 2021). Due to their persistence, toxicity and bioaccumulation potential, actions have been taken voluntarily by industries and regulators worldwide to reduce the release of PFAAs including PFOA, PFOS and perfluorohexane sulfonic acid (PFHxS) (Butenhoff et al., 2009; Wang et al., 2015; Wang et al., 2013). Legacy PFAAs have been replaced by shorter chain analogues (C3-C6) such as perfluorobutanoic acid (PFBA), perfluorobutane sulfonic acid (PFBS), and perfluorohexanoic acid (PFHxA) as well as perfluoroether carboxylic acids (Bao et al., 2018; Li et al., 2020; Wang et al., 2015). These replacement PFAS are considered less bioaccumulative but still have the potential to persist in the environment and are quickly becoming the dominant PFAS in aquatic ecosystems (Wang et al., 2015; Wang et al., 2013). For example in chemical and product manufacturing in the US, two of the replacement products for PFOA and PFOS are the hexafluoropropylene oxide dimer acid (HFPO-DA or GenX) and PFBS, respectively (U.S. Environmental, 2022a).

PFAS are also widely-documented in human plasma (Hu et al., 2019) and can be maternally transferred pre- and post-natal (Bach et al., 2016; Blake and Fenton, 2020). Some PFAS have also been linked with human developmental, metabolic, and immune disorders as well as certain types of cancers (Barry et al., 2013; Grandjean and Budtz-Jørgensen, 2013; Liu et al., 2018). Potential pathways to drinking-water resources are diverse, including biosolids application, outdoor products (e.g., ski waxes), industrial releases, firefighting foams, and discharges from wastewater treatment, septic, stormwater, and landfill systems (Houtz et al., 2013; Kurwadkar et al., 2022; Masoner et al., 2019; Masoner et al., 2020; Salvatore et al., 2022; Sims et al., 2022). PFAS have been detected globally in surface and groundwater drinking–water resources (Evich et al., 2022) and in public drinking–water supplies prior to distribution (Andrews and Naidenko, 2020; Domingo and Nadal, 2019; Hu et al., 2016; McMahon et al., 2022).

In the US, publicly–available large national (e.g., U.S. Environmental Protection Agency's Third Unregulated Contaminant Monitoring Rule (UCMR3) (U.S. Environmental Protection Agency, 2022b) and state-specific databases comprise results from samples collected from public drinking-water treatment plants after treatment and prior to distribution, an approach which does not account for distribution-system changes that can affect consumer exposures at the tap (e.g., (Chen et al., 2019; Li et al., 2022; Mohammadi et al., 2022). Currently, limited information exists on drinking-water PFAS concentrations at the point of exposure (i.e., point-of-use tapwater) in public-supply and especially in unregulated and generally unmonitored private-wells. Private-well owners make up about 13–14% of the US population (Dieter et al., 2018) and previous research has documented a range of contaminant concerns in unregulated/unmonitored private-well drinking-water (Bradley et al., 2021a; Charrois, 2010; Focazio et al., 2006). Because the burden of private-well maintenance and monitoring falls on the owner (U.S. Environmental Protection Agency, 2023c), private-well water quality information remains scarce and typically is limited to only a few contaminants (e.g., coliform bacteria), due to high analytical costs, confusion of aesthetic quality (taste, odor) with safety, and a range of socioeconomic factors (Seltenrich, 2017; Zheng and Flanagan, 2017). This circumstance leads to the increased probability of unrecognized contaminant exposures (Zheng and Flanagan, 2017) and adverse health effects to private-well dependents (American Academy of Pediatrics, 2009) and illustrates the continued need for comparable assessments in both private-wells and public-supply at the point-of-use. For PFAS, such assessments are essential for quantifying population-level drinking-water exposures, identifying at-risk or contaminated water sources or systems, and determining potential human-health implications, especially for vulnerable subpopulations (Andrews and Naidenko, 2020).

PFAS regulations are changing rapidly in the US as a growing number of increasingly strict state and federal drinking-water guidelines/benchmarks have been established over the last 20 years (Interstate Technology Regulatory Council, 2022; Post, 2021; U.S. Environmental Protection Agency, 2023b). However, there currently are no final enforceable national drinking-water standards (e.g., maximum contaminant level [MCL]) for PFAS in the US and some states over the last few years have adopted their own enforceable MCLs for several PFAS (Interstate Technology Regulatory Council, 2022). In March 2023 U.S. Environmental Protection Agency (EPA) released, for public comment, proposed MCLs of 4 ng/L and MCLGs (maximum contaminant level goal) of zero for PFOA and PFOS. MCLGs are non-enforceable health goals established to protect vulnerable subpopulations irrespective of treatment technology, cost, and limits of detection. Further, any contaminant considered a likely or known carcinogen receives an MCLG of zero (U.S. Environmental Protection Agency, 2023b). A hazard index approach was also proposed to regulate PFHxS, GenX, PFNA, and PFBS. This approach considers the health-based values for PFHxS (9 ng/L), GenX (10 ng/L), PFNA (10 ng/L), and PFBS (2000 ng/L) to determine if the combined individual hazard quotient values pose a potential risk (U.S. Environmental Protection Agency, 2023b; U.S. Environmental Protection Agency, 2020). Significant shifts in guidelines to be more stringent are due primarily to improved information on potential health effects and exposure of sensitive subgroups such as infants through drinking-water (Post, 2021) indicating the need for more robust regional and national assessments of drinking-water with an emphasis on downstream exposure at the point-of-use especially as new proposed MCLs are promulgated in the US.

The U.S. Geological Survey (USGS) has been conducting ongoing national research on the potential for human exposures (both home and workplace) from natural and man-made tapwater contaminants, including PFAS (Bradley et al., 2020; Bradley et al., 2018; Bradley et al., 2023a; Bradley et al., 2021a; Bradley et al., 2021b; Bradley et al., 2023b). To better understand human exposure to PFAS at the point-of-use, we conducted a standardized analytical survey of PFAS nationally using a network of volunteers and combined this new data with tapwater samples collected previously by our research team to maintain consistency in data collection/processing. The overall objectives of the study were to (1) directly compare PFAS exposure in regulated public-supply tapwater to tapwater from unregulated private-wells, (2) provide information on potential aggregated human-health effects of PFAS using health-based screening tools, and (3) identify potential landscape-scale drivers of PFAS contamination in tapwater.

2. Material and methods

2.1. Site selection and sample collection

This nationwide pilot assessment included 716 tapwater samples collected from residences, businesses, and drinking-water treatment plants across the US (Figure S1) from 2016 to 2021. Of these, 409 tapwater samples were collected at the point-of-use in 2021 from 155 unregulated private–well and 252 regulated public–supply locations in all 50 states, the District of Columbia, Puerto Rico, and the US Virgin Islands (Fig. 1, Figure S1) using a network of volunteers. Sampling locations were selected based on a presumptive–impact gradient approach wherein we identified locations in low (leveraged National Park Service/US Fish and Wildlife Service colleagues/sites), median (general outreach to colleagues and community volunteers, etc.), and high (targeted samples near reported PFAS sources based on geospatial information) human–impacted areas. Three locations (2 private-wells and 1 public-supply) were also sampled repeatedly (0, 0.5, 6, 12 and 24 h on day 1, daily for 7 days and then at least weekly for up to 2 months) to

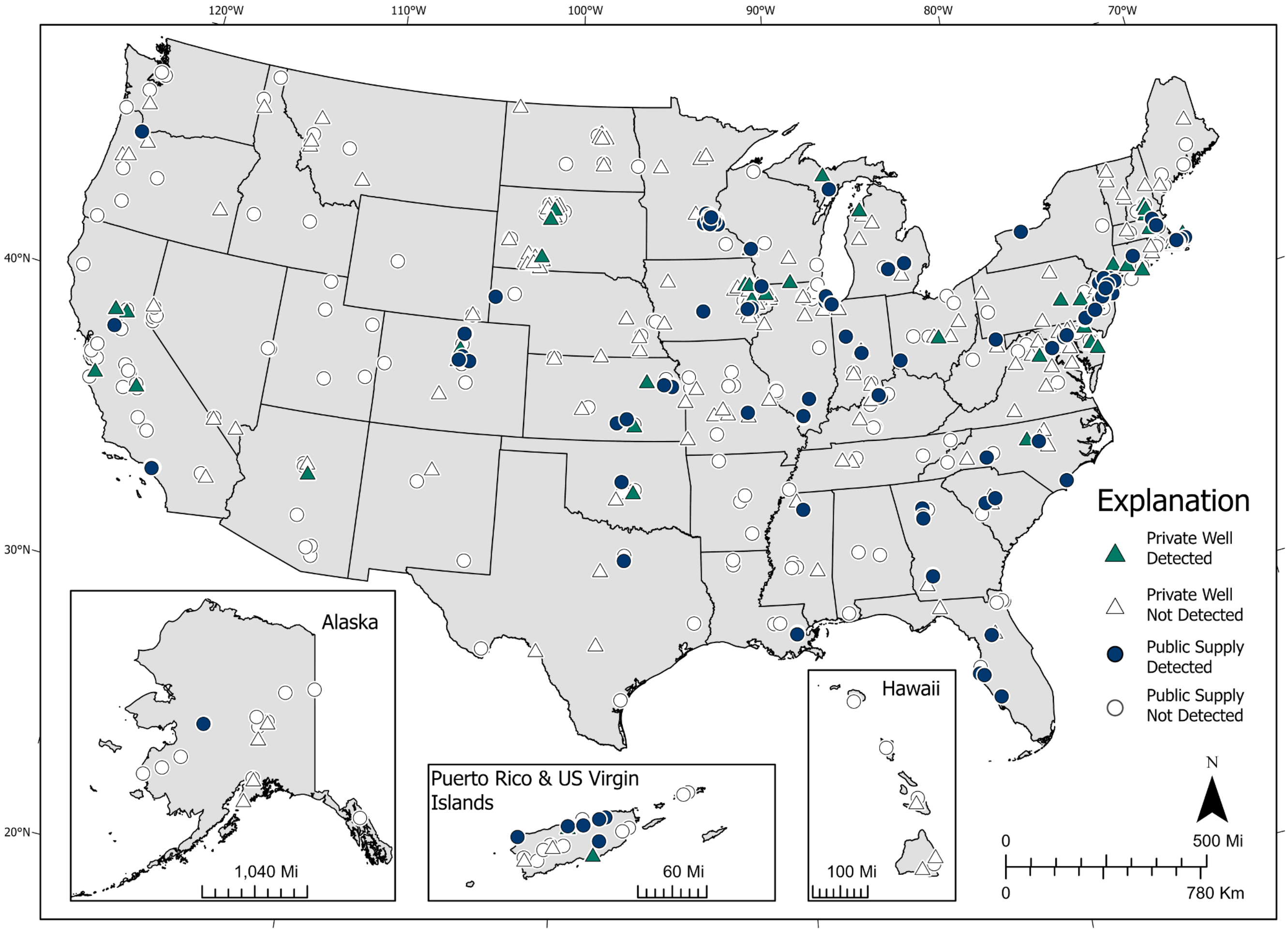

Fig. 1. Per- and polyfluoroalkyl substances (PFAS) detections in point-of-use tapwater collected from public-supply (blue circles) and private-wells (green triangles) across the United States including Puerto Rico and the U.S Virgin Islands. Samples with no detections are represented by open circles (public-supply) and triangles (private-wells). Tapwater samples were collected from 716 locations from 2016 to 2021. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

assess temporal changes in PFAS concentrations and profiles. Each volunteer was shipped a small cooler containing detailed instructions, and sampling supplies (gloves, two sets of three 2–mL polypropylene centrifuge tubes, and an ice pack). Instructions directed participants to rinse each tube three times, then fill half full, cap and chill until shipment. Samples were collected one time between July and December 2021 with sampling times varying throughout the day and without precleaning, screen removal or flushing of the sample tap. We requested samples from households without point of entry treatment and from faucets without a point-of-use treatment system (note, 1 location reported treatment after the sample was collected). All samples (three centrifuge tubes per sample) were collected in duplicate, and one set was frozen for archival.

PFAS data from an additional 307 tapwater samples (112 private-wells and 195 public-supply) collected as part of the USGS point-of-use tapwater research effort between 2016 and 2021 were also included herein (Table S1). USGS point-of-use tapwater research is conducted modularly with individual community-based studies (designed to address community priorities and support public-health decisions by individuals, communities, and public-health agencies) informing a national perspective in aggregate. Tapwater sampled in 2016 were collected in three 15-mL Falcon tubes, shipped on ice to the EPA National Exposure Research Laboratory (NERL) and extracted onto a solid phase extraction cartridge (SPE) prior to analysis based on methods described previously (Romanok et al., 2018c; Strynar, 2017; Strynar et al., 2015). Tapwater sampled 2017–2018 were collected in 15-mL Falcon tubes and shipped on ice to the Colorado School of Mines (CSM) laboratory where they were prepared for analysis based on previously published methods (Murray et al., 2019). All tapwater samples collected 2019–2021 were sent to the USGS National Water Quality Laboratory (NWQL) in three 2-mL polypropylene centrifuge tubes that had been rinsed three times prior to sampling, placed in a whirl pack bag and shipped on ice to the laboratory where they were stored frozen prior to analysis (Kolpin et al., 2021; Romanok et al., 2018c). Detailed information on previous study designs, site selection and sample collection are provided elsewhere (Bradley et al., 2020; Bradley et al., 2018; Bradley et al., 2021b; Bradley et al., 2022; Romanok et al., 2018c.

2.2. Analytical methods and quality assurance

Across all studies, PFAS were analyzed by three different laboratories: 1) EPA National Exposure Research Laboratory (NERL, 1 study, 26 samples) in 2016, 2) Colorado School of Mines (CSM, 3 studies, 82 samples) in 2017–2018, and 3) USGS National Water Quality Laboratory (NWQL, 6 studies, 608 samples) in 2019–2021, using previously published methods (Supplemental Information; Tables S1-S2). Potential effects (e.g., bias) associated with the use of different laboratories with varying detection limits and number/types of PFAS analyzed was addressed during statistical analysis.

The EPA NERL (Strynar, 2017; Strynar et al., 2015) method included the analysis of 10 PFAS that were first extracted onto a solid phase extraction (SPE) cartridge, eluted with methanol/ammonia solution and analyzed by ultra-high performance liquid chromatography (UPLC)-tandem mass spectrometry (MS/MS) operated in negative electrospray ionization (ESI) mode. The CSM method (Murray et al., 2019) included the analysis of 28 and 44 PFAS (Tables S2 and S3) using liquid chromatography quadrupole time-of-flight mass spectrometry (LC-QToF-MS) in negative electrospray ionization (ESI-) mode. The USGS method (Kolpin et al., 2021) included the analysis of 34 total PFAS (including PFOS and PFHxS reported separately as branched and linear) by matrix-modified samples and direct aqueous injection-liquid chromatography/tandem mass spectrometry (DAI-LC/MS/MS) with isotope-dilution quantification. Data were acquired in dynamic multiple reaction monitoring (dMRM) mode with two transitions per analyte for confirmation (except for PFBA and PFPeA that only had one confirming ion).

Method detection limits ranged from 0.1 to 61.8 ng/L depending on compound and laboratory (Table S3). Known bias associated with the variability in laboratory detection limits was accounted for in the selection of statistical models. Quantitative ($\geq$limit of quantitation (LOQ)) and semi-quantitative (between LOQ and long-term method detection limit, LMDL) results were treated as detections. Quality-assurance/quality-control included analyses of field blanks and stable isotope surrogates. The median surrogate recovery for PFAS across all studies and laboratories was 103% (interquartile range (IQR): 93–116%) and the median matrix spike recovery ($N = 84$) was 107% (IQR: 96–117%). For detailed information on PFAS recoveries by individual and study see Table S1 for links to all available data. Field blanks from the nine individual studies conducted 2016–2021 are detailed in the supporting information section and elsewhere (Bradley et al., 2020; Bradley et al., 2018; Bradley et al., 2023a; Bradley et al., 2021a; Bradley et al., 2021b; Bradley et al., 2022; Romanok and Bradley, 2021; Romanok and Bradley, 2018; Meppelink et al., 2022; Romanok et al., 2019; Romanok et al., 2018a; Romanok et al., 2018b; Romanok et al., 2023b; Romanok et al., 2023a; Romanok et al., 2022). For the new samples collected by our volunteer network, field blanks were collected by 47 volunteers selected at random from 37 states in 2021. PFBA was the only PFAS detected (one blank sample, 72.3 ng/L), resulting in the censoring of one value (52.1 ng/L) from the associated environmental sample (Romanok et al., 2023c).

2.3. Geospatial analysis

The geospatial analysis joined the 716 sample site locations with numerous geospatial layers and rasters to provide more detailed information regarding each sample site (Seawolf et al., 2023). The datasets included: sources listed in the EPA ECHO (Enforcement and Compliance History Online) Database as potential PFAS environmental release sites including broad categories such as airports, industry, waste management, oil and gas, and department of defense; land-use classes from both the National Land Cover Database (NLCD) and Coastal Change Analysis Program (C-CAP) (Seawolf et al., 2023; Multi-Resolution Land Characteristics Consortium, 2011; National Oceanic and Atmospheric Administration, 2022). A five-km spatial buffer was established around each sample site as a means of capturing the number of PFAS in close proximity to the sampling location and to calculate an average distance to source. Within that buffer each sample site was joined with proximal PFAS sources identified from the EPA ECHO dataset. This join resulted, for many sites included, in multiple potential PFAS sources proximal to each sample site.

We also performed a spatial analysis of the NLCD and C-CAP datasets around each sample site, collecting land use data within the five-km buffer. NLCD data from 2011 was used for both the continental US and Alaska. C-CAP data was available for the Hawaiian Islands. For the island of Hawaii, Maui, and Kuai we used C-CAP data from 2010. For the island of Oahu, C-CAP data from 2011 was used. C-CAP data from 2010 was used for the island of Puerto Rico and for the island of St. Thomas, C-CAP data from 2012 was used. Merging the C-CAP dataset with NLCD was not problematic. We followed the convention outlined in Table S4 to convert C-CAP classes to NLCD classes.

2.4. Statistical analysis

Three different Bayesian hierarchical statistical modeling approaches – employing different distributional assumptions – were used to accommodate the unique aspects of the three primary goals of the analysis. The modeling approaches included (1) a hierarchical regression model to accommodate left-censored observations (observations below detection limits) for individual PFAS (Qian et al., 2004; Wu et al., 2011); (2) a hierarchical Tweedie compound Poisson linear model to model the total PFAS data, which included skewed continuous observations of total PFAS concentrations and many sites with no PFAS detections (i.e., there is zero inflation); and (3) a hierarchical negative binomial regression to model the number of compounds detected at each site. Each of these three modeling approaches are discussed in more detail below and in the Supplemental Information section 1.2.

The Bayesian hierarchical approach to accommodating left-censored data that we employ is robust, and simulation studies have shown it performs well for recovering true contaminant distributions and can handle relatively high proportions of left-censored observations in the dataset (Qian et al., 2004; Stow et al., 2018). For each modeling approach, we fitted two models, a source model that evaluated potential differences between tapwater sources (private or public) and a geospatial model, in which some of the landscape properties hypothesized to influence PFAS concentrations and occurrence were included as predictor variables. For the source model, tapwater source was included as an indicator variable, with public-supply tapwater as the reference cell. For the geospatial models, we included those predictors that were not highly correlated with one another ($r < 0.60$). The final set of geospatial predictors included the proportion of total developed land, developed open land, cultivated agricultural land, and pasture agricultural land, along with the average distance to the nearest EPA ECHO site. All predictor variables were standardized (mean $= 0$, standard deviation $= 1$) prior to analysis. Because land use geospatial variables were highly skewed, they were logit-transformed prior to standardization. For individual PFAS analysis, we limited statistical analysis to those compounds that were measured above their respective detection limits in at least 5% of sites, resulting in inclusion of 8 compounds (PFBA, PFBS, PFHxA, PFHxS, PFOA, PFOS, PFPeA, PFPeS). We chose 5% of the sites as a cutoff because this provided enough observations that were recorded above the detection limit to allow for meaningful inferences of estimated parameters (i.e., lower than 5% resulted in very little information on concentrations above the detection limit to inform parameter estimates). The study, from which data were collected was included as a random effect in all models. All estimated parameters are reported using the posterior mean and 95% credible intervals (CRIs). The code for Bayesian model fitting and posterior inference is available at https://doi.org/10.5066/P9MCYEVS.

2.5. Screening-level assessment

A screening-level assessment (Goumenou and Tsatsakis, 2019; U.S. Environmental Protection Agency, 2011) of potential cumulative biological activity of available individual PFAS in each tapwater sample was conducted using two analogous bioactivity-weighted approaches (Σ_{EAR}, Σ_{TQ}) as described previously (Blackwell et al., 2017; Bradley et al., 2019; Bradley et al., 2018). The EAR approach is a considered a high-level screening of the potential for molecular-scale vertebrate effects to complement the Hazard Index (i.e., TQ) approach. The ToxCast vertebrate-centric *in vitro* effects library was specifically assembled to inform the potential for human biological effects (Blackwell et al., 2017). The ToxEval version 1.3.0 (De Cicco et al., 2018) was used to sum (non-interactive, concentration addition model, e.g., (Altenburger et al., 2018; Cedergreen et al., 2008; Stalter et al., 2020)) individual exposure activity ratios (EAR) from the Toxicity ForeCaster (ToxCast, high-throughput screening data (U.S. Environmental Protection Agency, 2022c) to estimate sample-specific cumulative EAR ($\sum$EAR) (Blackwell et al., 2017; Bradley et al., 2018). EAR is the ratio of the detected concentration in the sample to the activity concentration at cutoff (ACC) obtained from the ToxCast database. The ACC estimates the point of departure concentration at which a defined threshold of response (cutoff) is achieved for a given biological activity and is less prone to violations of relative potency assumptions (Blackwell et al., 2017). ACC data in the ToxEval v1.3.0 employed in the present study were from the August 2022 invitroDBv3.5 release of the ToxCast database including updated bioactivity information for individual PFAS (U.S. Environmental Protection Agency, 2022c). Non-specific-endpoint, baseline, and unreliable response-curve assays were excluded (Blackwell et al., 2017; Bradley et al., 2018). $\sum$EAR results are summarized in Table S10.

Because the $\sum$EAR approach was limited to 11 individual PFAS in ToxCast, an analogous human-health-based assessment (Goumenou and Tsatsakis, 2019; U.S. Environmental Protection Agency, 2012; U.S. Environmental Protection Agency, 2011) using available federal, state or international human-health benchmarks for 15 individual PFAS was also conducted to sum the toxicity quotient (TQ; ratio of detected concentration to corresponding health–based benchmark) of individual detections to estimate sample-specific cumulative TQ ($\sum$TQ) (Corsi et al., 2019). A precautionary screening–level approach was employed based on the most protective human-health benchmark (i.e., lowest benchmark concentration) available (Interstate Technology Regulatory Council, 2022). $\sum$TQ results and respective health–based benchmarks are summarized in Tables S10 and S5, respectively. Screening assessments were conducted in the program R version 3.6.1 (R Development Core Team, 2019). Differences (centroids and dispersions) among sample types (private-wells and public-supply) for Σ_{EAR} and Σ_{TQ} were assessed by one-way PERMANOVA ($n = 9999$ permutations) on Euclidean distance (Hammer et al., 2001).

3. Results and discussion

3.1. Spatial and temporal assessments of PFAS exposure in tapwater

In the US and globally, limited information is available on PFAS in point-of-use tapwater, with most drinking-water studies focused on samples from source waters (McMahon et al., 2022; Sims et al., 2022) or pre-distribution samples from community water supplies (Andrews and Naidenko, 2020; Hu et al., 2016; Kurwadkar et al., 2022; Li et al., 2022; McMahon et al., 2022; Neuwald et al., 2022; Post et al., 2013), largely omitting distribution system factors (e.g., plumbing material with PFAS or sorption/degradation in the supply network; (Mohammadi et al., 2022) and a notable paucity of data available for private-wells across the US. To address this gap, we utilized targeted analysis of up to 44 PFAS in point-of-use tapwater from 269 private-wells and 447 public-supply collected 2016–2021 as fractional indicators of the presumptive 8000 + PFAS contaminant (U.S. Environmental Protection Agency, 2022a) (Fig. 1, Figure S1, Table S1). Consistent with other studies and large datasets focused on public–supply tapwater (Hu et al., 2016; Li et al., 2022; McMahon et al., 2022; Post et al., 2013), at least one PFAS was observed in 30% (237 of the 716) of the tapwater samples collected throughout the US (Fig. 1, Figure S2). Based on data from the UCMR3, about 4% of US drinking-water treatment plants tested had detectable PFAS but the breadth of contamination was likely missed due to high detection limits (10–90 ng/L depending on individual PFAS) and a limited number of PFAS analyzed (Hu et al., 2016). More recently, assuming lower detection limits, Andrews and Naidenko (2020) estimated that approximately half the US population likely receive water with PFOA/PFOS concentrations<1 ng/L, but this information has yet to be validated fully with field data particularly at the point-of-use. In our study, seventeen PFAS were detected at least once and, apart from perfluoropropane sulfonic acid (PFPrS), all detected PFAS were analyzed in > 600 samples (Table S2). Reporting limits for the PFAS observed in the current study varied by laboratory and ranged from 0.1 to 20 ng/L (Table S3). The most frequently detected PFAS analyzed by all laboratories included PFBS (16%), PFHxS (15%), and PFOA (14%), similar to results reported by others for drinking-water resources (surface water intakes or groundwater wells) or community water supplies (Andrews and Naidenko, 2020; Boone et al., 2019; McMahon et al., 2022; Post et al., 2013; Teymoorian et al., 2023). The number of individual PFAS observed ranged from one to nine (median of two) with detected concentrations ranging from 0.025 to 319 ng/L (median: 2.88 ng/L) and corresponding cumulative PFAS concentrations (sum of 16 detected PFAS) ranging from 0.348 to 346 ng/L (median: 7.00 ng/L; Table S10). As expected, sites classified as 'low' impact had the lowest prevalence of PFAS compared to sites near known PFAS sources, whereas PFAS varied widely among sites classified as 'medium.'.

At least one PFAS was detected in 20% of private-well (55/269) and 40% of the public-supply (182/447) samples collected throughout the US. A similar pattern was reported in groundwater from the eastern US, in which 60% of the public-supply wells and 20% of monitoring wells contained at least one PFAS (McMahon et al., 2022). Median cumulative PFAS concentrations (estimated considering detection limits and including study as a random effect) were comparable between public-supply (median = 7.1 ng/L [95% CRI = 2.3, 17.1]) and private–well point-of-use tapwater (median = 8.2 ng/L [95% CRI = 2.6, 20.5]; Fig. 2). Similarly, considering only PFAS with > 5% detections, we observed no differences in estimated median concentrations of individual PFAS or in the number of detected individual PFAS between public-supply and private-well point-of-use tapwater samples (Fig. 2, Tables S7-8). We chose 5% as a cutoff because this provided enough observations above the detection limit to allow for meaningful inferences of estimated parameters. Based on model predictions (Figure S3), the probability of not detecting PFAS above our detection limits ranged from approximately 25% in urban centers (e.g., Chicago) or areas with a known history of PFAS contamination (e.g., Cape Cod (Bradley et al., 2021a)) to > 75% in rural areas (e.g., Northern Plains (Bradley et al., 2022)). Figure S3 illustrates the spatial (among-study) variability that exists in PFAS occurrence (and concentration, not shown) quantified by the study random effect included in all models to account for variability in detection limits and the difference in numbers of PFAS included in each method (Tables S7-8, S10-11). Across all studies, the probability of detecting one PFAS was approximately 18%, with a marked decrease in probability with increasing number of detected compounds; no differences were observed between public-supply and private-well samples (Fig. 3).

Due in large part to funding constraints and prioritization of population-relevant reconnaissance of a range of exposure points within a given community, point-of-use tapwater exposure studies conducted to date (Bradley et al., 2020; Bradley et al., 2018; Bradley et al., 2023a; Bradley et al., 2021a; Bradley et al., 2021b; Bradley et al., 2023b) typically have employed a one-time spatial–synoptic approach, which provides limited to no insight into point-of-use tapwater temporal variability. To address this data gap, PFAS samples were collected temporally at 3 of the residential locations (2 private-wells, 1 public-supply). The rural, private–well location in South Carolina had no PFAS detected during three months of sampling. PFAS were detected at the suburban public-supply and private-well locations in New Jersey, and cumulative detected concentrations were generally stable (hourly increasing to weekly samples) over 3 months (Figures S4, S5). In light of the near-detection-limit concentrations of several individual PFAS detections, the observed variabilities in detections of some individual PFAS and in per-sample cumulative PFAS detections (Figure S4) were likely due more to method–sensitivity limitations (Teymoorian et al., 2023) than to short-term changes in drinking-water resources. New Jersey (NJ), one of the more proactive states regarding PFAS regulation, has established enforceable NJ-MCLs for three PFAS including PFOA (14 ng/L), PFNA (13 ng/L) and PFOS (13 ng/L) (New Jersey Department of Environmental Protection, 2022a) and has added PFOA, PFOS and PFNA

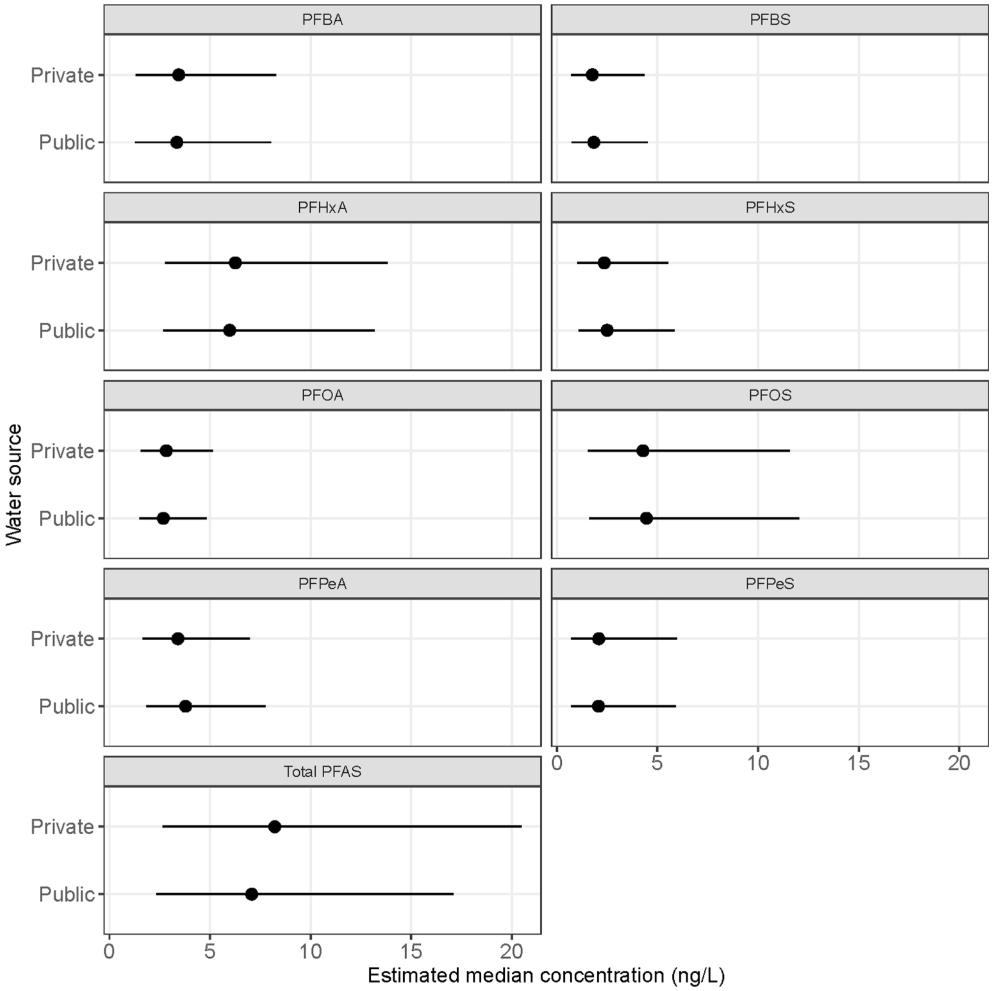

Fig. 2. Estimated median concentrations (ng/L) of select per- and polyfluoroalkyl substances (PFAS) and cumulative PFAS in private-wells and public-supply samples. Circles are posterior means and horizontal lines are 95% credible intervals.

to the Private-well Testing Act, which requires homeowners to test potable wells prior to sale and landlords to test their well water and report results to the tenant once every five years (New Jersey Department of Environmental Protection, 2022b). None of the detections in either location exceeded NJ-MCLs. These results further support the need for continued monitoring of PFAS in point-of-use tapwater from residential private-wells as well as for continued temporal assessments to accurately assess PFAS exposures at the point-of-use more broadly.

3.2. Comparison to proposed US drinking water regulations

Newly proposed MCLs for PFOA (4 ng/L) and PFOS (4 ng/L) were released in March 2023 by EPA as part of the National Primary Drinking-water Standards Rule (U.S. Environmental Protection Agency, 2023b). The proposed MCL for PFOS was below the reporting limit for two of the three laboratories (CSM:1.3 ng/L, NERL: 5.0 ng/L and USGS: 7.4 ng/L; Table S3) used during this study; consequently, our estimates of samples exceeding the proposed MCL should be considered conservative. The reporting limit for PFOA was above the proposed MCL for only one laboratory (CSM: 1.3 ng/L, NERL: 5 ng/L, USGS: 2.0 ng/L; Table S3) in which the least number of samples were analyzed (26/716; Table S1). Proposed MCLs for PFOA and PFOS were exceeded in 6.7% and 4.2%, respectively, of all tapwater samples collected but were exceeded in 48% (48 of 99) and 70% (30 of 43), respectively, of tapwater samples when detected. Further, proposed MCLs for PFOA and PFOS were exceeded in 63% and 67%, respectively of the private-well tapwater samples and in 44% and 77%, respectively of the public-supply tapwater samples, when detected. The proposed MCLG (zero) (U.S. Environmental Protection Agency, 2023b) was de facto exceeded in every sample in which PFOS and PFOA was detected (private-well: 15 and 24, respectively; public-supply: 28 and 75, respectively). Further, to account for dose additive noncancer effects of PFBS, PFNA, PFHxS, GenX, EPA proposed an MCL for the mixture of these four PFAS based on a hazard index approach (U.S. Environmental Protection Agency, 2020). The proposed hazard index of 1 for the sum of the toxicity quotient (measured concentration/health-based value) for PFBS + PFNA + PFHxS + GenX was exceeded in 4.6% of tapwater collected.

3.3. Aggregated screening-level assessments

We also used two bioactivity weighted screening approaches Σ_{EAR} and Σ_{TQ} to provide insight into the potential aggregated (sum of all PFAS) effects. These approaches are limited by the availability of weighting factors (ToxCast ACC and health-based benchmarks, respectively) and mixture effects are estimated by assuming concentration addition (Cedergreen, 2014). The Σ_{EAR} approach has been used effectively in other studies as a protective (conservative) screening tool to asses drinking-water exposure risk to organic contaminant mixtures because it leverages response relations for>9000 organic chemicals across over 1000 standardized vertebrate cell lines (Kavlock et al., 2012; Kavlock et al., 2008; Richard et al., 2016). Contaminant bioactivity ratios were aggregated across all ToxCast endpoints available for

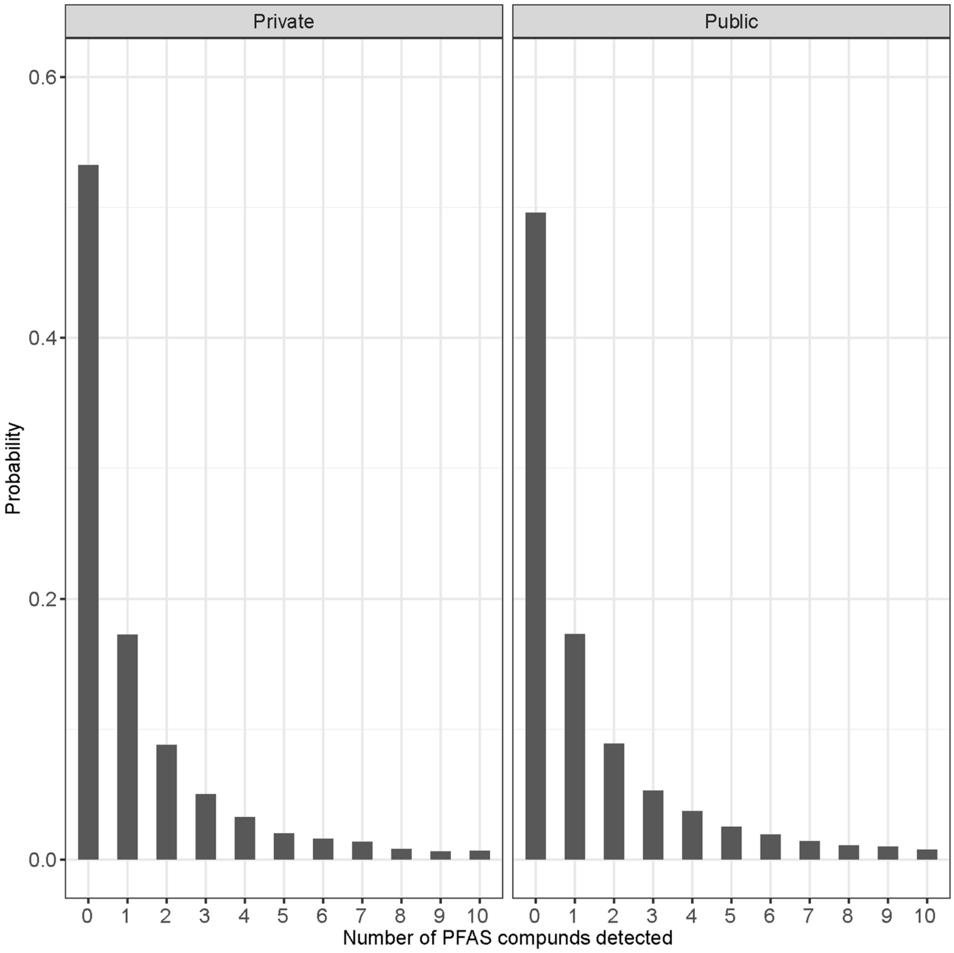

Fig. 3. The predicted posterior probability of detecting 1 – 10 per- and polyfluoroalkyl substances (PFAS) in private-well and public water-supply tapwater.

individual PFAS without restriction to recognized modes of action to provide a precautionary lower-bound estimate of in vivo adverse-effect levels (Paul Friedman et al., 2020), however, this approach may not accurately reflect apical effects (Blackwell et al., 2017; Schroeder et al., 2016). Further, for PFAS, the approach has the potential to underestimate exposure risk because only 11 of the detected compounds had exact Chemical Abstract Services number matches in the ToxCast™ database and only six (PFOS, PFOA, PFNA, PFHpA, PFBA, PFHxS) of these had EAR exceeding our lowest threshold for consideration (>0.00001). The $\sum_{TQ}$ approach targets apical human-health effects, is notably constrained to recognized (i.e., benchmarked) health concerns and was used herein to estimate cumulative effects from a broader suite of PFAS (15 with established health-based benchmarks; Table S5) (Interstate Technology Regulatory Council, 2022). Lastly, it is important to note, the EAR approach is based on measured endpoint-specific activity cutoff concentrations, whereas the human-health benchmarks used in the TQ approach generally include a margin of safety (margin of exposure).

None of the samples exceeded a $\Sigma_{EAR} > 1$, a value which indicates cumulative exposure at concentrations capable of modulating molecular endpoints *in vitro,* and we observed no systematic differences in Σ_{EAR} between private–well and public–supply locations (Fig. 4). However, 65 tapwater samples exceeded the $\Sigma_{EAR} = 0.001$ precautionary screening level of potential concern (yellow line, Fig. 4; Table S10) for molecular effects described previously (Bradley et al., 2018). For PFAS and PFOA, which proposed MCLGs of zero, EPA's interim health advisory levels released in 2022 (U.S. Environmental Protection Agency, 2022a) were used as the benchmark value (Table S5). Σ_{TQ} values were higher in private–well tapwater samples compared to public–supply ($p = 0.0015$), and 124 samples overall had $\Sigma_{TQ} > 1$ (Fig. 4, Table S10), indicating a high probability of aggregated risk when considering exposures to all observed PFAS with an available benchmark. As expected, given their proposed MCLG of zero (U.S. Environmental Protection Agency, 2023b), Σ_{TQ} results were driven by PFOA and PFOS, when detected. Simultaneous detection of multiple PFAS is consistent with other drinking-water (Andrews and Naidenko, 2020; Boone et al., 2019; Hu et al., 2016) and tapwater studies (Bradley et al., 2020; Bradley et al., 2018; Bradley et al., 2021b) in the US. The results of precautionary Σ_{EAR} and Σ_{TQ} assessments by this group indicate that the potential for human-health effects from contaminant exposures (including PFAS) through drinking-water are common and comparable in private-well and public-supply tapwater (Bradley et al., 2020; Bradley et al., 2018; Bradley et al., 2021a). Information generated by this study and elsewhere indicates the need for further assessments of cumulative health exposure risks of PFAS mixtures (Kwiatkowski et al., 2020) and of PFAS in combination with other organic and inorganic contaminants of concern, particularly in unmonitored/unregulated private-wells where information is limited or not available.

3.4. Predicting exposure based on potential sources and land-use

The final model comparing tapwater PFAS concentrations to geospatial drivers included median distance to potential source (including airport, industry, waste management, oil and gas, and department of defense) and several land-use classifications (total developed, open developed, cultivated and pasture agriculture). The number of PFAS sources in a 5–km buffer around each site was highly correlated with developed land-use ($r = 0.66$) and was excluded from the model.

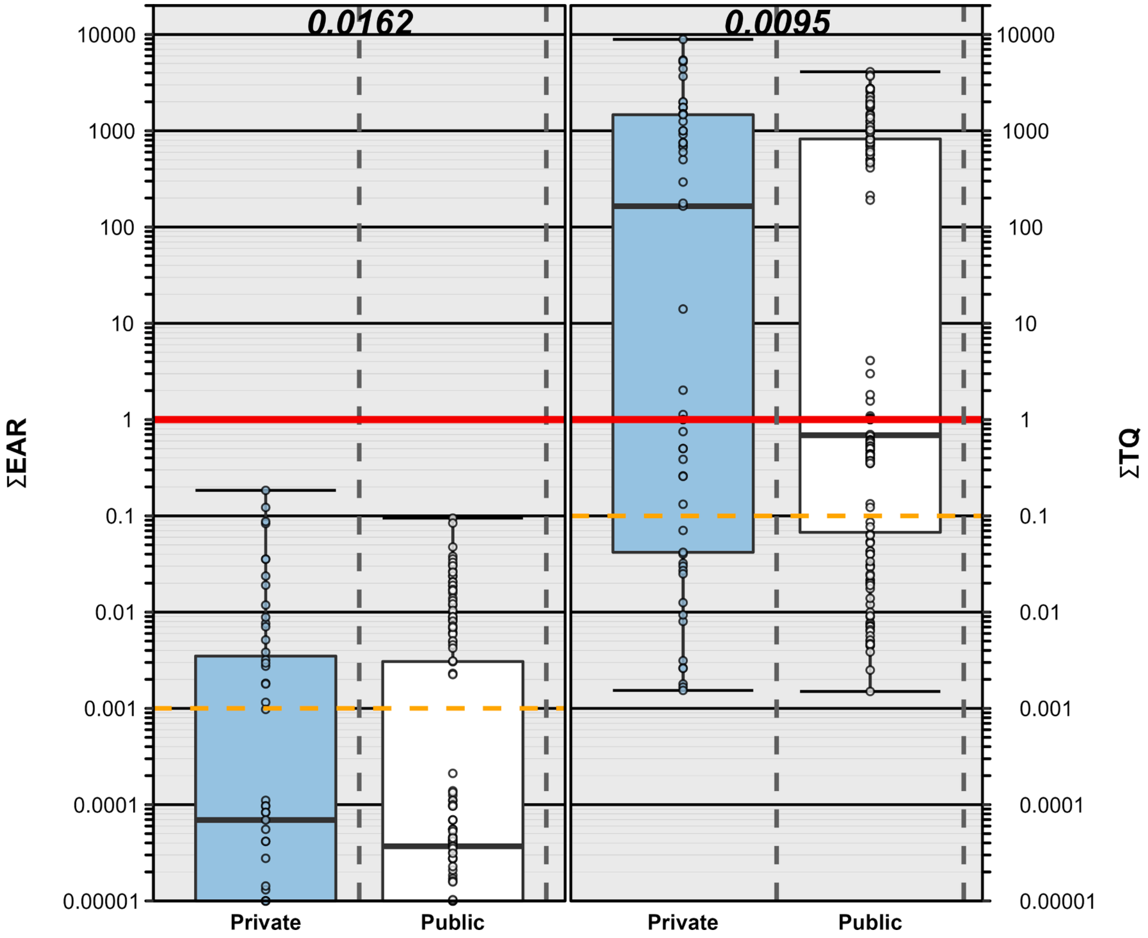

Fig. 4. Left. Cumulative maximum Exposure-Activity Ratios (∑EAR) across all assays for 9 individual per- and polyfluoroalkyl substances (PFAS) in ToxCast and detected in tapwater collected from public-supply and private-wells. Solid red and yellow lines indicate concentrations shown to modulate effects *in vitro* and effects-screening-level thresholds (EAR = 1 and EAR = 0.001), respectively. Right. Human-health benchmark cumulative toxicity quotient (ΣTQ) for 15 PFAS listed in Table S5 and tapwater from public-supply and private-wells. Solid red and yellow lines indicate benchmark equivalent concentrations and effects-screening-level threshold of concern (TQ = 0.1), respectively. Boxes, centerlines, and whiskers indicate interquartile range, median, and 5th and 95th percentiles, respectively. Numbers above each boxplot pair indicate the permuted probability that the centroids and dispersions are the same (PERMANOVA; 9999 permutations). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Cumulative PFAS concentrations and the number of detected compounds increased with surrounding developed–land and decreased with increasing distance from probable source(s) (Fig. 5, Figure S6, Tables S10-11). However, for individual PFAS the distance to probable source(s) was not a strong predictor of concentration (Figure S7, Table S8). PFBS was the only PFAS which exhibited a positive relation with development and pasture agriculture and a negative relation with open development (commonly includes large-lot single-family housing units, parks, golf courses, and vegetation planted in developed settings for recreation, erosion control, or aesthetic purposes). Although biosolids application is a recognized source of PFAS to surface- and groundwaters in agricultural landscapes (Munoz et al., 2022; Sepulvado et al., 2011), in this study concentrations of PFBS, PFHxA, PFHxS, PFOA and PFOS decreased with increasing surrounding cultivated cropland. Further, for several compounds (PFBA, PFHxA, PFHxS and PFOA), concentrations decreased with increasing development, an unexpected result which suggests that point-of-use tapwater exposure to individual PFAS in our study is more closely associated with the type of PFAS sources (e.g., industry, airport, wastewater, etc., which are generally located at the edge of urban development and not in the highest residentially-developed areas) (Hu et al., 2016) rather than numbers of potential PFAS sources (Salvatore et al., 2022). Because our geospatial analysis was constrained to broad putative-source categories (e.g., military fire training areas, industrial, wastewater) and 90% of the corresponding potential sources were characterized as industrial, exploration of source-type/point-of-use tapwater exposure relationships was limited and merits further investigation. Further, most public-supply samples were collected at the tap not the treatment facility, indicating a distinct disconnect from PFAS source and drinking water resource. Despite these limitations, the real–world point-of-use tapwater PFAS concentration data compiled herein along a national gradient of presumptive contamination represents an important validation dataset to assess and tune putative-source PFAS contamination models, like that presented recently (Salvatore et al., 2022).

3.5. Implications and future directions

Approximately 40 million people in the US rely on private-wells for drinking-water (DeSimone et al., 2015; Dieter et al., 2018), most national testing programs, like the UCMR3 focused on community water supplies serving ≥ 10,000 consumers, do not include private-wells and rarely capture information from rural communities (52 million people rely on small water supplies serving < 10,000), indicating data on PFAS exposure and potential human-health effects is does not exist for over one-third of the US population (Hu et al., 2016). As noted previously, small public supplies and private-wells may be disproportionally affected by PFAS, emphasizing the value of studies like these focused broadly on point-of-use tapwater PFAS exposures, with an emphasis on

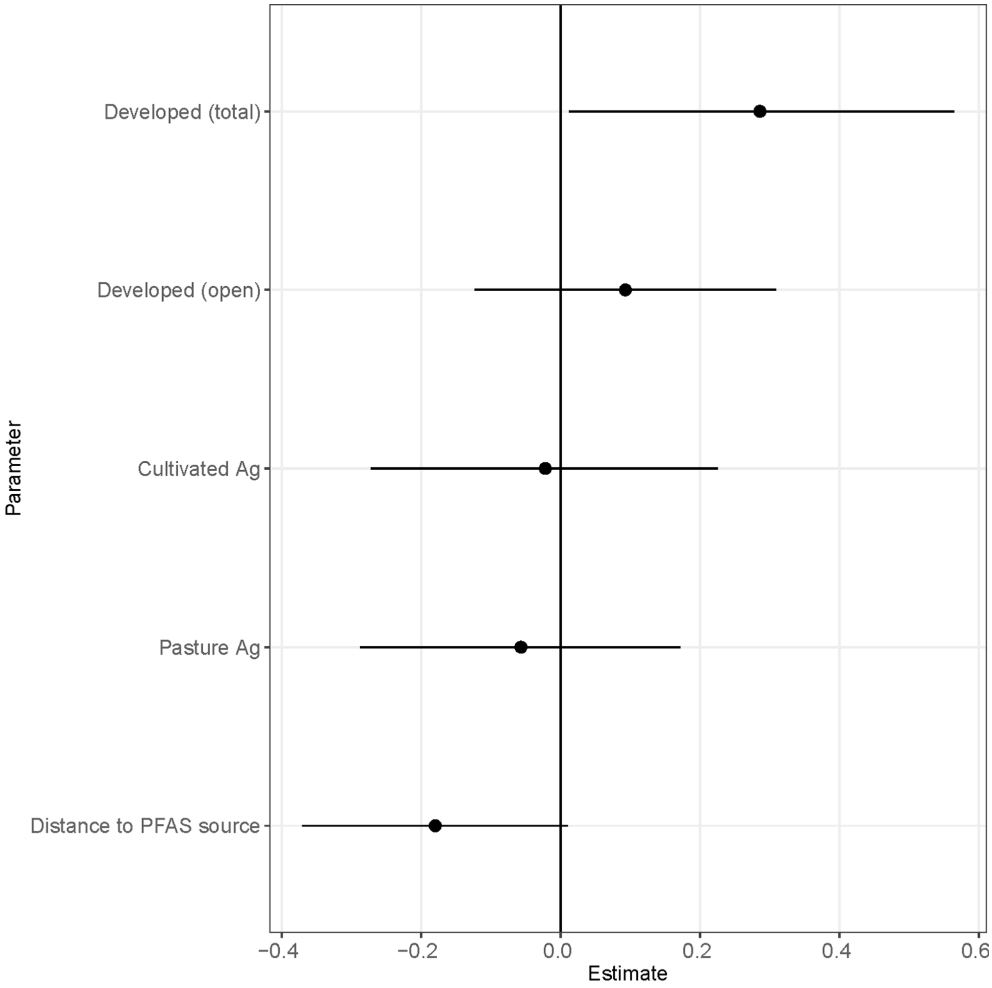

Fig. 5. Estimated effects of geospatial predictor variables on cumulative per- and polyfluoroalkyl substances (PFAS) concentrations. Circles are posterior means and horizontal lines are 95% credible intervals. Geospatial predictors with 95% credible intervals that overlap with zero are not considered statistically significant.

comparing exposures in private-wells with those directly from public-supply using similar sampling/analytical methods. Some of these gaps associated with PFAS in small community public supply facilities may be addressed by the UCMR5, currently underway in the US and expected to provide extensive information on PFAS in US drinking water for public-supply consumers in the next few years (U.S. Environmental Protection Agency, 2023a).

Modeled results indicate that on average at least one PFAS is detected in about 45% of US drinking-water samples. Results also indicate that 1) detection probabilities vary spatially (8% in rural areas up to > 70% in urban areas/areas with a known history of PFAS contamination), 2) drinking-water exposures may be more common in the Great Plains, Great Lakes, Eastern Seaboard, and Central/Southern California regions, and 3) temporal variations in concentrations/detections may be limited. Geospatial datasets and land-use information were correlated with both cumulative PFAS concentrations, and the number of PFAS detected; however, they were not often correlated with specific PFAS profiles due to the limited number of individual PFAS detected more than once using targeted approaches. Targeted PFAS analytes are only a fractional indicator of the 8000 + potential PFAS and the fraction of total organic fluorine captured by these targeted analyses is typically low in surface water (D'Agostino and Mabury, 2017; McDonough et al., 2019) and drinking-water (Jiao et al., 2022). Potential detection of one or more PFAS in US drinking-water combined with the paucity of information available on current use/ultra-short chain compounds (Neuwald et al., 2022) supports the continued need for point-of-use tapwater monitoring, with an emphasis on unmonitored private-wells and underserved communities on small community water supplies. To fully understand exposure and adequately determine risk to human-health, continued emphasis should be placed on 1) integrating geospatial datasets with PFAS data broadly to identify vulnerable regions/subpopulations, 2) expanding monitoring to include rural small–system and private–well dependent communities, and 3) expanding target and non-target analysis methods particularly in drinking-water monitoring programs in the US and globally.

CRediT authorship contribution statement

Kelly L. Smalling: Conceptualization, Formal analysis, Investigation, Methodology, Project administration, Visualization, Writing – original draft, Writing – review & editing. **Kristin M. Romanok:** Data curation, Formal analysis, Investigation, Methodology, Visualization, Writing – review & editing. **Paul M. Bradley:** Formal analysis, Investigation, Methodology, Project administration, Writing – review & editing. **Mathew C. Morriss:** Investigation, Writing – review & editing. **James L. Gray:** Investigation, Writing – review & editing. **Leslie K. Kanagy:** Investigation, Writing – review & editing. **Stephanie E. Gordon:** Investigation, Visualization, Writing – review & editing. **Brianna M. Williams:** Investigation, Visualization, Writing – review & editing. **Sara E. Breitmeyer:** Visualization, Writing – review & editing. **Daniel K. Jones:** Writing – review & editing. **Laura A. DeCicco:** Investigation, Writing – review & editing. **Collin A. Eagles-Smith:** Investigation, Writing – review & editing. **Tyler Wagner:** Investigation, Formal analysis, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

All data are available. All data presented can be found in a series of USGS data releases (Meppelink et al., 2022; Romanok and Bradley, 2018; Romanok and Bradley, 2021; Romanok et al., 2022; Romanok et al., 2019; Romanok et al., 2023a; Romanok et al., 2023b; Romanok et al., 2023c). For links to the individual USGS data releases see Table S1.

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Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envint.2023.108033.

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STATE OF NEW MEXICO
DEPARTMENT OF ENERGY, MINERALS AND NATURAL RESOURCES
OIL CONSERVATION COMISSION

IN THE MATTER OF PROPOSED
AMENDMENT TO THE COMMISSION'S
RULES TO ADDRESS CHEMICAL DISCLOSURE
AND THE USE OF PERFLUOROALKYL AND
POLYFLUOROALKYL SUBSTANCES AND
THEIR USE IN OIL AND GAS EXTRACTION,
19.15.2, 19.15.7, 19.15.14, 19.15.16 AND 19.15.25 NMAC **CASE NO. 23580**

SELF-AFFIRMED STATEMENT OF JANET ANDERSON

1. My name is Janet Anderson and I am employed by GSI Environmental Inc. as a Vice President and Principal Toxicologist. My responsibilities include providing consulting support to clients on technical issues related to toxicology, risk assessment, risk communication, and risk management. I am familiar with WildEarth Guardians' (WEG) August 23, 2024, Amended Application for Rulemaking (Application), the proposed amendments to the referenced rules as provided in the Exhibit to the Application, and the proposed modifications filed by the New Mexico Oil and Gas Association (NMOGA).

2. My educational background and my work experience is accurately summarized in **[NMOGA Exhibit E1]**. I believe my credentials qualify me to testify as an expert witness in Oil Conservation Commission Case No. 23580.

3. I have been asked by NMOGA to address WEG's proposed amendments to the Commission's rules 19.15.2, 19.15.7, 19.15.14, 19.15.16, 19.15.3.25 NMAC to address per- and polyfluoroalkyl substances (PFAS) in oil and gas extraction. In connection with my testimony I will introduce and discuss **NMOGA Exhibits E2**

NMOGA Exhibit E

through E29. These exhibits were either prepared by me or compiled under my direction and supervision.

INTRODUCTION

4. WEG's Application included a (1) written statement outlining WEG's reasoning for requesting the amendments to the above-listed rules; (2) WEG Exhibit 1, which is a copy of existing regulations with WEG's proposed changes in redline; and (3) WEG Exhibit 2, a proposed Public Notice for the rulemaking.

5. PFAS are a large class of highly diverse, man-made chemicals that have been around since the 1950s, and which, generally speaking, contain carbon-fluorine bonds, instilling substances with stability, resiliency, and inertness. PFAS have been used in various industrial and consumer applications, and include polymers and non-polymers; solids, liquids, gases; and persistent and nonpersistent substances (Buck et al., 2011), **[NMOGA Exhibit E2].**

- Regulatory and public health concerns regarding potential human and environmental risks associated with PFAS began in the late 1990s and early 2000s following disclosures from a PFAS manufacturer that certain PFAS (the "long chain" non-polymer perfluoroalkyl acids, perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS)) were detected at a high occurrence in their occupational worker serum, serum samples from the general public, and environmental samples from remote locations.
- Since then, the research and regulatory attention on PFOA, PFOS, and similar non-polymer PFAS has grown rapidly. These two compounds, PFOA and PFOS, in particular, raise concerns due to their environmental

persistence and high frequency of detection, extremely long retention time in the human body, occurrence in >95% of the general population's blood, and wide range of potential health effects.

- Depending on how the term PFAS is defined (explained further below), this class of compounds may include between a few hundred to more than 10,000 chemicals. However, importantly, not all of these chemicals have these same physical, chemical, or toxicological characteristics.
- Some PFAS are not environmentally persistent.
- Some PFAS are not water soluble or considered mobile in the environment.
- Some PFAS are rapidly eliminated from the human body.
- Some PFAS are inert polymers.
- And some PFAS do not have an association with a wide range of potential human or ecological health effects, although robust toxicological information on the majority of PFAS is lacking.

AMENDED APPLICATION FOR RULEMAKING

6. In its Application, WEG states that "PFAS are an exceptionally toxic group of chemicals that present myriad, long-term, and persistent public health and environmental hazards." (p. 1). This statement is factually inaccurate and misleading.

- The term "PFAS" represents a diverse and large class of chemicals, with extremely diverse physicochemical characteristics, fate and transport, and potential human and ecological toxicity. As stated in the Organisation for Economic Co-operation and Development (OECD) report "Reconciling

Terminology of the Universe of Per- and Polyfluoroalkyl Substances: Recommendations and Practical Guidance":

> *"The term "PFASs" does not inform whether a compound is harmful or not, but only communicates that the compounds under this term share the same trait for having a fully fluorinated methyl or methylene carbon moiety. … It should be noted that "PFASs" is a broad, general, non-specific term, which should only be used when talking about all the substances included in the PFAS definition described here (or the user should clearly define the scope of which substances are being referred to as PFASs in the documents they prepare). Otherwise, it would introduce ambiguity and even factual error in the statements (as occurred sometimes in past literature)."* (OECD, 2021, p. 32), **[NMOGA Exhibit E3].**

- The WEG statement that PFAS are "exceptionally toxic" cannot be applied to this broad group of chemicals.
- Some compounds broadly identified as PFAS (i.e., compounds that contain a single fully fluorinated methyl or methylene carbon moiety) are routinely used as pharmaceuticals, prescribed to children and adults, such as Lipitor, Flonase, Paxlovid, and Prozac, and are often prescribed with dosing regimens that maintain long-term exposure levels but have

been deemed safe for human use. (For example, see (Hammel et al., 2022), **[NMOGA Exhibit E4]**; (Pennoyer et al., 2023), **[NMOGA Exhibit E5].**

- Some PFAS, such as the fluoropolymers including polytetrafluoroethylene (PTFE), are not water soluble and would not be expected to be found widespread in groundwater. (Henry et al., 2018), **[NMOGA Exhibit E6]**; (Korzeniowski et al., 2022), **[NMOGA Exhibit E7].**
- Most of the chemicals identified as PFAS have little to no toxicity data available, which makes it impossible to claim that any of these compounds are "exceptionally toxic". The U.S. Environmental Protection Agency (USEPA) states:

  > *"Although certain PFAS, such as perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS), have been studied extensively, most PFAS lack data for robustly characterizing their potential toxicity."* (USEPA, 2021b), **[NMOGA Exhibit E8].**

- Even for the PFAS that are similarly grouped in the subfamily of fully fluorinated, non-polymer chemicals with available toxicity data (PFOA, PFOS, perfluorononanoic acid (PFNA), perfluorobutanoic acid (PFBA), perfluorohexane sulfonate (PFHxS), etc.), have different identified potential health effects (e.g., thyroid disruption versus cancer), different potencies, and very different toxicity profiles. (For example, *see* (Goodrum et al., 2021)), **[NMOGA Exhibit E9].** Therefore, even among this small subset, it is incorrect to assume that these PFAS present the same potential risk, and it is incorrect to assert that all PFAS are "exceptionally toxic".

- For example, perfluorooctadecanoic acid (PFODA), a fully fluorinated, non-polymer PFAS, currently has a residential tap water screening level from the USEPA of 800 micrograms per liter (µg/L), which is over 100 million times higher than the screening level for PFOA of 2.7×10^{-6} (µg/L).[1] These two PFAS have vastly different toxicities and, therefore, regulatory screening levels and should not be assumed to be the same.
- Furthermore, PFAS as a class are not all associated with "multiple health effects including cancer," as WEG claims in its Application (p.2).
- Only PFOA and PFOS are listed as "likely to be carcinogenic to humans" by the USEPA (USEPA, 2024b), **[NMOGA Exhibit E10];** (USEPA, 2024a), **[NMOGA Exhibit E11]**. The Agency has evaluated the toxicity datasets for numerous other PFAS, including PFNA, perfluorobutane sulfonic acid (PFBS), PFBA, PFHxS, perfluorohexanoic acid (PFHxA), and hexafluoropropylene oxide (HFPO-DA, also called GenX) and none of the currently available datasets revealed these PFAS to be carcinogenic.
- WEG's factually inaccurate statement that all "PFAS" are "exceptionally toxic" only serves to confuse and mislead the Oil

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[1] USEPA screening levels for resident tap water available: https://www.epa.gov/risk/regional-screening-levels-rsls-generic-tables. Accessed September 10, 2024.

Conservation Commission (OCC) and the public regarding these chemicals.

- For this reason, the term "PFAS" should be more specifically enumerated and must delineate between PFAS for which there is toxicology data and potential concerns for human health risks and those PFAS for which no such data or concerns exist. Statements regarding potential human or environmental risk must be limited to the compounds for which data are available to inform what exposure levels may present an unacceptable increase in risk, on a chemical-specific nature.

7. WEG, in its Application, also cites a 2021 report by the Physicians for Social Responsibility (PSR or PSR Report) that claims to "confirm the presence of PFAS in oil and gas hydraulic fracturing operations." (Horwitt & Physicians for Social Responsibility, 2021), **[NMOGA Exhibit E12]**. I, and other GSI colleagues, previously wrote a rebuttal to the claims in the PSR Report. This rebuttal is included herein (Connor et al., 2021), [**NMOGA Exhibit E13]**.

- According to the PSR Report, evidence suggests that PFAS have been used in hydraulic fracturing for oil and gas operations, and this use "is another potential route of exposure to PFAS." (Horwitt & Physicians for Social Responsibility, 2021), **[NMOGA Exhibit 12]**. They further state that this use could potentially contaminate "a huge amount" of water or soil and "could pose a risk" if this fluid was spilled, dumped as wastewater, burned via flaring, or impacted sources of residential tap water.

- Importantly, 94% of the instances where the PSR Report identified that PFAS were reportedly used as a liquid additive for fracturing fluid occurred prior to 2017 (Connor et al., 2021), **[NMOGA Exhibit 13]**. Moreover, of the nearly 184,000 records on hydraulic fracturing projects in FracFocus nationwide, only approximately 1,600 report the use of PFAS in hydraulic fracturing fluids, which represents less than 0.9% (1,600/184,000) of the hydraulic fracturing projects on record (Connor et al., 2021), **[NMOGA Exhibit 13]**. In other words, over 99% of hydraulic fracturing projects on record have used no such additives. Finally, the PSR report does not provide any data to support the WEG statement that "The use of PFAS by the oil and gas industry leads to the creation of PFAS-contaminated produced water and other nondomestic waste." With many thousands of hydraulic fracturing projects completed in the US, there is no evidence of "already impacted regions," where hydraulic fracturing has impaired groundwater or surface water, as stated by PSR (Connor et al., 2021), **[NMOGA Exhibit 13]**. Thus, WEG's assertion that the PSR Report "confirms the presence of PFAS in oil and gas hydraulic fracturing operations" overstates and misstates the actual conclusions that can be drawn from the data analyzed.

19.15.2.7 DEFINITIONS

8. In WEG Exhibit 1, WEG proposes to amend the definitions to the regulations to add eight (8) new defined terms to 19.15.2.7 NMAC. I address certain proposed changes to add definitional terms below.

9. “Chemical” – WEG provides a novel definition of “chemical,” as “any element, chemical compound, or mixture of elements or chemical compounds that has a specific name or identity, including a Chemical Abstracts Service number.” (p.7). As proposed, this definition is both unnecessary and technically confusing. First, WEG’s definition of “chemical” is circular (i.e., includes the word “chemical” in the definition). Second, because the suggested revisions to the regulations are aimed at PFAS, it is unclear why “chemical” as a general term needs to be defined herein.

- Chemicals are matter composed of a defined combination of atoms that have mass and volume, and often have specific Chemical Abstracts Service (CAS) numbers.
- Consequently, WEG’s proposed “chemical” definition is irrelevant to a rulemaking addressing PFAS specifically; confusing because of its circuitousness; and contrary to what is scientifically the common understanding of the term, “chemical.” The OCC should not adopt WEG’s definition of “chemical,” as proposed in 19.15.2.7.

10. “PFAS Chemicals” – WEG provides a redundant and circular definition of PFAS. WEG has defined “PFAS chemicals” as “perfluoroalkyl or polyfluoroalkyl substance with at least one fully fluorinated carbon atom.” (p. 9).

- The term “PFAS” is an acronym for per- or polyfluoroalkyl substances. Simply stating that PFAS means “perfluoroalkyl” and “polyfluoroalkyl substance” is, again, circular. As discussed above, the term PFAS does not have a consistent, agreed-upon definition, and using the term without a more precise and technically accurate definition can introduce technical ambiguities and factual errors. Furthermore, other regulations addressing the definition of "PFAS" have limited PFAS to substances with two or more sequential fully fluorinated carbon atoms in the defined term "PFAS."

- For consistency with other existing regulations, I recommend using a definition that aligns with the USEPA regulatory Toxic Substances Control Act definition of PFAS (USEPA, 2024c), **[NMOGA Exhibit E14]**. Therefore, PFAS should be defined as follows: **PFAS are substances with two or more sequential fully fluorinated carbons.** Such a definition is generally consistent with the existing USEPA definition and is also technically sound, as enumerated below.
- Substances containing a single isolated $–CF_2–$ are likely to degrade and are not considered persistent. Compounds with only a single $–CF_3$ (i.e., only the terminal carbon is fluorinated) are commonly used in pesticides and pharmaceuticals, each of which have their own extensive regulatory safety programs and chemical-specific toxicological profile evaluations prior to commercial use. Consequently, neither single isolated CF_2s nor CF_3s are proper to include within the definition of PFAS in this rulemaking, which addresses PFAS in downhole oil and gas operations, not those PFAS used in pesticides, pharmaceuticals, or other commercial applications. Thus, revising the definition of "PFAS" to be "**substances with two or more sequential fully fluorinated carbons**" is both consistent with existing federal regulations defining the PFAS and is

supported by the science on PFAS. Furthermore, defining PFAS in this manner addresses those chemicals potentially relevant to oil and gas operations and includes the PFAS with data available to assess potential human and/or environmental impacts (i.e., human and ecological toxicity data for risk assessments).

- Given the common use of PFAS in a variety of products and substances (Buck et al., 2011), **[NMOGA Exhibit E2]**, most of which are unrelated to downhole oil and gas operations, and "background levels" of some PFAS (for example see, (Vedagiri et al., 2018), **[NMOGA Exhibit E15]**; (Zhu et al., 2022), **[NMOGA Exhibit E16]**, I also recommend that the revised language include "intentionally added" as part of the definition for "PFAS."
- "Intentionally added PFAS" means **PFAS that have been deliberately added to a product to impart a functional or technical effect on the product.**
- The OCC should, accordingly, adopt a definition for PFAS as follows: "**PFAS are intentionally added substances with two or more sequential fully fluorinated carbons.**" The OCC should not adopt the definition of PFAS that WEG proposes at 19.15.2.7 NMAC, which is inconsistent with federal regulations and unsound from a technical and scientific point of view, as discussed above.

19.15.16.17 COMPLETION OPERATIONS, SHOOTING AND CHEMICAL TREATMENT OF WELLS

11. In 19.15.16.17(A)(4), WEG inserts new proposed text that reads, "[i]f testing reveals the presence of PFAS or undisclosed chemicals, the Division may revoke authorization to operate upon consideration of whether the current operator or previous well owners' operations contributed to the *presence* of PFAS or undisclosed chemicals." (p. 14) (emphasis added). WEG's proposed addition to 19.15.16.17(A)(4) is inappropriate and contrary to federal and state best standard practices for chemical risk assessment.

- The central tenet of toxicology and risk assessment is that "the dose makes the poison." The mere *presence* of a chemical does not constitute a risk to human or environmental health. For a chemical that is present in the environment to present an unacceptable risk, it: (1) has to be present both at a level that has the potential to cause adverse effects and there (2) has to be a potentially complete exposure pathway (i.e., a route of exposure for the chemical starting in the environmental media to the receptor, such as groundwater used for drinking water).
- This central tenet of toxicology is why threshold levels for chemicals in drinking water or any environmental media are developed by regulatory and public health agencies. Detection of a chemical alone is insufficient to trigger follow-up action.
- Rather, consideration of complete exposure pathways and the concentration level of a specific chemical in a given media are critical to the evaluation of potential risk and/or follow-on actions.

- The concept of chemical risk assessment that includes chemical-specific dose-response toxicity information and an exposure assessment to inform risk management decision-making is well-established by international, federal, and state authorities, including the New Mexico Environment Department (NMED) (for example, see: (NRC, 1983), **[NMOGA Exhibit E17]**; (NRC, 1994), **[NMOGA Exhibit E18]**; (USEPA, 1989), **[NMOGA Exhibit E19]**; (UESPA, 1997), **[NMOGA Exhibit E20]**; USEPA, 1999), **[NMOGA Exhibits E21].**
- NMED has detailed explicit guidance regarding the use of risk assessment standard methods for environmental site investigations and guiding remediation. NMED guidance includes consideration of exposure pathways and assumptions, chemical-specific and physical-chemical parameters, and potential background (i.e., non-site related) levels (NMED, 2017), **[NMOGA Exhibit E22]**; **(**NMED 2022), **[NMOGA Exhibit E23].**
- Requiring follow-on regulatory action from the mere "*presence* of PFAS or undisclosed chemicals" *alone* without any evaluation of whether (1) the aforementioned are present at a level that has a potential to cause adverse effects; or (2) there is a potential exposure pathway is contrary to well-established scientific principles of risk assessment and tenets of toxicology. The OCC should not adopt 19.15.16.17(A)(4) as WEG has modified this regulation.

19.15.16.19 LOG, COMPLETION, AND WORKOVER REPORTS

12. (D) Disclosure. WEG's requested revisions to 19.15.16.19(D) includes a requirement "to provide the chemical disclosure list," (with "chemical disclosure list" being a newly defined term in 19.15.2.7(C) under WEG's proposed revisions) to a large list of entities and individuals, including, but not limited to, building owners, residents, tribal members, schools, government actors, and public water system administrators. (pg. 15).

13. This proposed disclosure requirement does not serve to improve public health. In fact, requiring disclosure in the manner WEG contemplates in the proposed revised 19.15.16.19(D) could cause unnecessary distress to the public because the manner of such disclosure is inconsistent with and, in some instances, contrary to, standard risk communication best practices.

- Proper public risk communication regarding chemicals potentially present in the environment is essential to avoid "chemophobia," which is known to result in a decrease in public health, and other social and economic adverse effects (e.g., diversion of resources, mistrust of government and/or industry, increased anxiety and stress in communities (Entine, 2011), **[NMOGA Exhibit E24].**
- It is often assumed that presenting the public and stakeholders with factual information is always in the public's best interest and the stakeholders will be readily able to develop appropriate "beliefs, attitudes and behaviors related to a given risk." (USEPA, 2021a),

[NMOGA Exhibit E25]. However, according to the USEPA, research has shown this not to be true. (USEPA, 2021a), **[NMOGA Exhibit E25]**.

- The entities included on WEG's Disclosure list in 19.15.16.19(D) do not have the training or experience to distinguish between "safe" and "unsafe" substances present in the environment. As described above, a risk assessment is the standard of practice to determine potential public health risk; the mere presence of a chemical does not equate to an unacceptable risk to human health or the environment, as discussed above.
- There are numerous examples of unjustified public hysteria over the misinterpretation that the mere presence of a chemical directly results in detrimental effects on human health and the environment. (see for example discussion in (Entine, 2011), **[NMOGA Exhibit E24])**.
- There are also examples of determinantal effects on public health related to the misinformation and fear associated with chemicals in the environment, rather than associated with the adverse health effects of the chemicals themselves. (Calloway et al., 2020), **[NMOGA Exhibit E26]**.
- The National Academies of Science recognizes that psychological stress is an important consideration when studying environmental health risks, (NRC, 2009), **[NMOGA Exhibit E27]**, and stress itself has been shown to contribute to adverse human health conditions including cardiovascular issues and immune responses. (Reviewed in (Calloway et al., 2020), **[NMOGA Exhibit E26].**

- An unfortunate extreme example of the fear and stress caused by potential environmental exposure is the Flint Michigan water crisis, wherein the prevalence of depression and posttraumatic stress disorder symptoms were still elevated in the community regardless of actual lead exposure concentrations (Brooks & Patel, 2022), **[NMOGA Exhibit E28]**. In other words, the designation of living in a community with contaminated water and the perceived risks had measurable negative public health outcome irrespective of the actual levels of lead in the community water.
- To best manage and to minimize psychological distress and unnecessary public fear, public disclosure regarding the potential presence of environmental chemicals needs to follow well-established risk communication strategies.
- The USEPA defines "risk communication: as the process of informing people about potential hazards to their person, property, or community" (ITRC, 2020), **[NMOGA Exhibit E29]**. Following standard best practices for risk communication has "a clear impact on whether an audience can hear, understand, accept and act on a specific message." (USEPA, 2021a), **[NMOGA Exhibit 25]**.
- As explained in the Interstate Technical and Regulatory Council (ITRC) risk communication guidance, presenting information regarding chemicals in the environment is challenging and complicated. Stakeholders will want to know if the presence of a chemical will cause

or has caused health impacts, and explaining this requires explaining scientific concepts such as complicated chemistry, fate and transport, health effects, exposure information, and knowledge gaps (ITRC, 2020), **[NMOGA Exhibit 29]**.

- As such, disclosure of the potential presence of a list of various chemicals in the environment does not serve to support improved public health unless the presence of each chemical on any such list is put into the context of technical information including which chemicals specifically the disclosure covers, the concentration(s) of each chemical listed, fate and transport of each chemical, potential for human exposure to each chemical, and potential specific adverse health effects from each chemical. Importantly, without this additional technical detail, no stakeholder will be equipped to understand possible risks or make appropriate risk management decisions based on or as a result of the chemical disclosure that WEG proposes in 19.15.19(D).
- Moreover, disclosing information in the manner WEG suggests, that is, through an enumerated list of chemicals without any context, could cause unnecessary health effects, including, but not limited to, psychological effects. The OCC should not adopt 19.15.16.19(D) as WEG has proposed in this modified regulation.

CONCLUSION

14. In my opinion, the proposed changes regarding the definitions of "chemical" and "PFAS" should not be adopted. The proposed provision should be modified to remove the unnecessary and circular definition of "chemical" and should adopt a definition consistent with the USEPA regulatory definition of "PFAS". This definition should also include "intentionally added" to avoid the unintended consequences related to low-level "background" detections of certain PFAS commonly found throughout the environment. Additionally, the proposed changes regarding the mere presence of PFAS should be removed, and instead, the standard practice of considering risk (that is, considering chemical-specific exposure pathways and levels) should be incorporated, consistent with other New Mexico regulations. Finally, the proposed language requiring disclosure of chemicals should be removed, as this requirement is unlikely to meaningfully improve public health or regulatory decision-making without the necessary context of data interpretation and risk assessment.

15. I affirm under penalty of perjury under the laws of the State of New Mexico that the foregoing statements are true and correct. I understand that this self-affirmed statement will be used as written testimony in this case. This statement is made on the date next to my signature below.

Janet Anderson
Janet Anderson

10/21/2024____
Date

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Janet K. Anderson, PHD, DABT

Vice President / Principal Toxicologist

Dr. Janet Anderson is a Principal human health toxicologist and risk assessor with over 15 years of experience providing toxicology expertise and consultation to federal agencies, municipalities, and private industry. She specializes in the synthesis of human health toxicology data into regulatory and legislative policies that govern environmental risk, product stewardship, and public health protection. With a comprehensive background in evaluating the toxic properties of emergeing and legacy chemicals, she works to ensure that scientifically informed processes are utilized in decision-making. She conducts site-specific risk assessments, including for CERCLA sites and environmental justice settings, and also provides litigation consulting support and has served as an expert witness.

Dr. Anderson is a nationally recognized leader in unregulated and emerging chemicals, such as per- and polyfluoroalkyl substances (PFAS), 1,4 dioxane, microplastics, and 1,2,3-trichloropropane. With in-depth knowledge of federal and state environmental guidance and policies pertaining these chemicals, she has developed strategies to mitigate potential human health impacts and address associated business risks for both private and public sector clients. She tracks the dynamic regulatory changes for emerging chemicals in the U.S. and internationally, offering clients the technical basis for disparate guidelines worldwide. She also has extensive experience developing corporate risk management strategies for emerging and legacy chemicals, as well as providing clients with due diligence support concerning potential liability across the full life-cycle of product manufacturing, use, and disposal.

Dr. Anderson is a diplomate of the American Board of Toxicology and an active member of the Society of Toxicology. A skilled communicator, she is often an invited speaker at high-level scientific conferences, regulatory meetings, webinars, and community stakeholder meetings. She excels at translating complex risk, regulatory, and public health information to different audiences and stakeholders.

PROJECT EXPERIENCE

Emerging Chemicals Strategies and Management

PFAS Product Liability and Reporting Requirements, Confidential Clients. Provide technical support regarding current supply chain and component parts use of PFAS. Review product literature and related manufacturing information. Support client team with regulatory updates and technical expertise related to PFAS chemistries, uses, and regulations.

PFAS Site Assessments, Confidential U.S. and International Sites. Provide technical support regarding historic and current Aqueous Film-Forming Foam (AFFF) storage and operations and potential environmental concerns. Develop

NMOGA Exhibit E1

detailed site assessment report that consolidates and summarizes available relevant site-specific information and current local regulatory landscape with regard to PFAS and AFFF use.

PFAS Product Stewardship and Environmental Support, Confidential Client. Provide technical support related to product manufacturing formulations, use, occupational exposures, potential environmental releases, and changing U.S. and European regulations for a current fluoropolymer industry user.

Regulatory Tracking and Analyses, United States. Serves as a regulatory toxicology subject matter expert for emerging chemicals such as PFAS and 1,4-dioxane. Is responsible for tracking the toxicological data and regulatory assessments and decisions internationally; providing summaries and impact assessments for clients; engaging with regulatory authorities to ensure sound scientific basis of regulatory decisions; and advising and developing risk management strategies to minimize effects of changing information and regulations, to ensure public and employee safety and health. Numerous clients.

Development of PFAS Source Differentiation Guidelines for Airports, for the National Academies of Science, Transportation Research Board. Serves as the Primary Investigator leading the technical team's development of a guidebook and technical resources related to PFAS forensic analysis for airport environmental managers. (ACRP 02-91)

Due Diligence Support for Mergers and Acquisitions, Confidential Clients. Provides technical support concerning potential PFAS liability associated with historic and current business practices and products in support of merger and acquisition due diligence.

Strategic Support Related to Management of Aqueous Film Forming Foam (AFFF) Use and Replacement. Provides confidential client with state-of-the-science updates and technical support related to regulatory and human health/environmental risks associated with AFFF use at oil and gas facilities.

Technical and Regulatory Support for the National Association for Surface Finishing. Provides technical consulting support, including toxicology, exposure, chemistry, training, and science communication, to, and on behalf of, the metal and surface finishing industry within the United States. Represents client in regulatory and legislative meetings and ensure that the human and environmental risks associated with metal plating processes is accurately understood and communicated to internal and external stakeholders.

Risk Communication and Regulatory Support Related to Contamination of Public Drinking Water, Confidential Municipality, U.S. Provides technical and strategic regulatory toxicology risk communication support to a U.S. drinking water municipality with unregulated and emerging chemicals present in source water. Ensures the municipality understands the human health risks and regulatory actions. Represents client in regulatory, and public meetings and ensure that toxicology and human health risk information is accurately communicated to and by stakeholders.

Risk Communication and Regulatory Support, 1,4-Dioxane. Confidential Publicly Owned Landfill, U.S. Provides regulatory toxicology, site-specific risk assessment reviews, and risk communication support to a publicly owned landfill with 1,4-dioxane in leachate. Ensures the human health risk assessments and regulatory actions are technically sound.

State-by-State Survey, United States. Participated in a survey of state and federal regulatory programs and initiatives to assess the level of activity and process by which emerging chemicals, such as PFASs, are prioritized and regulated. Analyses include understanding how state regulatory and public health agencies identify, prioritize, and develop strategies and standards to manage emerging chemicals. Work resulted in a compendium of all state-level initiatives related to emerging chemicals, which allows users to understand trends and state-specific interests.

Emerging Issues and Contaminants Program Management, U.S. Air Force Civil Engineer Center, Lackland, Texas. Served as program manager of an emerging contaminants program with a $1.2 million annual budget. Oversaw support contractors, wrote documents, delivered presentations, led internal management briefings, and led department training sessions. Identified gaps in scientific knowledge that underlies USAF and DOD efforts to protect human and environmental health. Specific topics included vapor intrusion, PFAS, 1,4-dioxane, chlorinated solvents (trichloroethylene, tetrachloroethylene) and pesticides. Also monitored evolving regulatory and political arenas to identify changes that could impact environmental cleanup costs, schedules, and procedures and policies. Developed programmatic recommendations for budget and resource needs to address environmental regulations and cleanup standards.

Risk Communication, U.S. Air Force Civil Engineer Center, Lackland, Texas. Provided risk communication materials such as factsheets and informational seminars to the general public interested in understanding PFAS site-specific environmental risk and cleanup strategies affecting their community. Served as technical support to USAF public affairs officials working within a community directly impacted by PFAS-contaminated drinking water. Crafted risk communication tools and products coordinated public meetings and agenda topics, and ensured that complex toxicology information was translated appropriately to the public.

Litigation Expert and Consulting Services

Expert Service, 1,4-Dioxane Cancer Risk, Long Island, New York. On behalf of Dow Chemical Company, Ferro Corporation, Vulcan Materials Company provide expert witness and consulting services related to 1,4-dioxane cancer risk assessment and mode of action. *Suffolk County Water Authority v. The Dow Chemical Company, Ferro Corporation, Vulcan Materials Company, Procter & Gamble Company, Shell Oil Company, individually and doing business as Shell Chemical LP.* Case No. *17-cv-6980.*

Expert Services, PFAS and Disinfection By-products Exposure and Risk, Tallassee, Alabama. On behalf of Tallassee Waste Disposal Center, Inc. provide expert witness and consulting services in connection with purported PFAS and disinfection by-products in plaintiffs' drinking water. *Leroy Taylor v. Advanced Disposal Services South, LLC et al. In the Circuit Court of Macon County, Alabama* Case No. *46-CV-2017-900075* (and related cases).

Expert Services, Aqueous Film Forming Foam (AFFF) and PFAS Toxicological History and Regulations. On behalf of the U.S. Department of Justice, Environmental & Natural Resources Division, provide consultation and expert opinion on the regulatory and human health toxicological history of AFFF and PFAS. *(Penna v. The United States of America, in the United States Court of Federal Claims,* Case No. 16-1545L).

Expert Services, Carbon Monoxide, California. On behalf of ITW Food Equipment Group, LLC, served as expert testifying witness on the regulatory toxicity values for, and process for human health risk evaluation of, carbon monoxide. (*Julie Lee, Julie Lacey, Lourdes Munoz, Martha Silva, Brandon Adams, Lafayette Wallace, Joshlynn Jarboe, Yolanda Rodriguez, Peter Lee and Mark Rodriguez v. Hobart Corporation, Wayne Home Equipment, A Scott Feitzer Co., A.M. Wighton & Sons, Inc., DBA A&J Refrigeration. In the Superior Court of Santa Barbara, Cook Division, California,* Case Number: 1389541).

Expert Services, 1,2,3-Trichloropropane, California. On behalf of Shell and Dow Chemical Co., served as expert on the use and interpretation of regulatory standards and toxicity values for 1,2,3-trichloropropane. (*City of Arcadia v. The Dow Chemical Company et al., In the U.S. District Court, Central District of California,* Case Number: 2:18-cv-10139, and related cases.)

Expert Services, Dieldrin and Aldrin, Florida. On behalf of Shell Oil Company, served as expert testifying witness and authored a detailed expert report on the regulatory toxicity values for, and human health risk evaluation of, dieldrin and aldrin. (*Janice Potter, Brian Potter, David Stepp, Debra Stepp, Renee Bolton, Yvonne Hopp, Herman*

Osterloh, Morgan Canada and Lauren Kelly, Class Representatives v. Shell Oil Company and DeLand Golf Course, Inc. In the Circuit Court, Seventh Judicial Circuit, in and for Volusia County, Florida, Case Number: 2011-11036-CIDL Division).

Expert Services, Portland, Maine. On behalf of Mallinckrodt U.S., LLC, served as expert testifying witness regarding human health risks and related remedial action of methylmercury in biota and sediments in the Lower Penobscot River and Estuary. *(Natural Resources Defense Council et al. v. HoltraChem Manufacturing Company, LLC et al., U.S District Court, District of Maine,* Civil Action No. 1:00-cv-00069-JAW*).*

Litigation Support Services, Alaska. On behalf of Williams Alaska Petroleum, provided technical support to the testifying expert on the appropriate toxicity values for site-specific risk assessment on sulfolane. (*State of Alaska et al. vs. Williams Alaska Petroleum et al., Shook, Hardy, and Bacon In the Superior Court for the State of Alaska Fourth Judicial District Court,* Case No. 4FA-14-01544CI).

Consulting Support Services, p-Chlorobenzenesulfonic Acid Contamination. For a confidential client, provided regulatory support and toxicology assessment.

Dispute Resolution, U.S. Air Force, Lackland, Texas. Provided technical support to USAF legal offices and program managers engaged in federal and state dispute resolution related to emerging issues and contaminants, including trichloroethylene, tetrachloroethylene, 1,4-dioxane, and perfluorinated compounds.

Toxicology

Toxicology Dossier for FluoroProducts and PFAS for Europe (FPP 4EU), Belgium. On behalf of Cefic's FPP 4EU group, principal investigator leading the collection and summary of information relevant to the human and ecological toxicity of select polymer and nonpolymer PFAS. Information is used to support European Union Chemicals Agency evaluation of PFAS for proposed regulations.

Expert Panel - PFAS Immunotoxicity Review, SciPinion. Support an expert panel evaluation of PFAS immunotoxicity data (epidemiology, laboratory animal) for human health risk assessment. Compiled introductory summary information, guided the panel through deliberations, and supported the development of manuscript documenting findings and recommendations.

Expert Panel Lead - PFAS Grouping Strategies, SciPinion. Led an expert panel evaluation of PFAS grouping strategies for human health risk assessment. Compiled introductory summary information, guided the panel through deliberations, and lead the development of manuscript documenting findings and recommendations.

PFAS Product Stewardship, United States. Provide technical support on short-chain PFAS and related fluorochemical products to the American Chemistry Council. Conduct scientific assessment related to the health and environmental risk of short-chain PFAS and fluorotelomers.

Technical Peer Review of Federal and State Agency Guidance Documents, United States. Provides technical peer review of toxicology assessments, risk assessments, and guidance documents on behalf of clients, including peer reviews of EPA IRIS and Toxic Substances Control Act (TSCA) assessments, ATSDR toxicological profiles, California Office of Human Health and Environmental Assessment documents, and other state regulatory agency assessments. Numerous clients and chemicals.

Nickel Proposition 65 Strategy and Support. Worked with the Nickel Institute to develop guidance related to compliance with the California Proposition 65 requirements for nickel and nickel compounds.

Technical Review and Comment on the New York Department of Health Proposed Rulemaking for 1,4-Dioxane Maximum Contaminant Level (MCL) (I.D. NO. HLT-30-19-00006-P). Conducted a review of the current toxicological data related to 1,4-dioxane's carcinogenic human health risks and authored a comment letter to the New York State Department of Health on the technical validity of their proposed MCL.

Short-chain PFAS and Fluoropolymer Toxicology and Regulatory Support, United States. Provides toxicology support to a confidential client working to obtain regulatory approval for current PFAS-containing products.

Federal Toxicology and Risk Assessment Reviews, United States. Served as a member of the federal interagency review team providing consultation and expert review on nearly all toxicology assessments and/or guidance documents produced by EPA, NTP, and ATSDR. Assessed the technical validity, transparency of decisions, adherence to agency and other federal guidance, and overall technical competency of the risk assessments. Work included submitting detailed written comments and participating in interagency teleconferences and working meetings.

Technical Review and Comment on the New Jersey Drinking Water Quality Institute (DWQI) Maximum Contaminant Level Recommendation for 1,2,3-Trichloropropane (1,2,3-TCP), New Jersey. Conducted a critical review of the toxicology, epidemiology, toxicokinetic, and other studies relevant to 1,2,3-TCP human health effects. Technical comments are part of the administrative record and continue to be considered by DWQI.

Technical Review of Pentachlorophenol Epidemiology Data in Response to Proposed California Proposition 65 Listing, California. Provided critical review and analysis of the developmental and reproductive epidemiology data on pentachlorophenol in response to the California Developmental and Reproductive Toxicant Identification Committee review and proposed listing under Proposition 65.

Toxicology Evaluation of Remedial Action Objectives, California. Conducted an in-depth assessment of outdated remedial action objectives for a confidential contaminated site in California. Reevaluated the toxicology and quantitative risk assessment for a specific unregulated contaminant of concern at the site. Calculated new screening levels based on updated risk assessment methodologies to ensure that remediation actions remain protective of public health.

Human Health Chemical Hazard Identification and Dose-Response, Federal Agencies, Cincinnati, Ohio. Provided management and scientific expertise for chemical assessments performed under Superfund, IRIS, and other programs. Served on high-performance, interdisciplinary scientific teams for dioxin reassessment, computational toxicology, phthalate cumulative risk, and mode of action.

Human Health Risk Assessent (HHRA)

CERCLA Baseline Human Health Risk Assessment for PFAS, former Wurtsmith Air Force Base, Oscoda, Michigan. Serves as principal in charge and technical lead for the PFAS baseline human health and ecological risk assessment at the former installation. Supports the USAF and state agency discussions, developed the conceptual site model, selection of toxicity values, and exposure pathways and parameters for human health risk characterization.

CERCLA Baseline Human Health and Ecological Risk Assessments for PFAS, Hoosick Falls, NY. Serves as project manager and technical lead for a PFAS baseline human health and ecological risk assessment at a National Priority List site in EPA Region 2. Developed regulator-approved Work Plans, including conceptual site models, toxicity information, exposure pathways and parameters for assessing human and ecological receptor exposures. Leading a team of multi-disciplinary scientists through the data review and evaluation, technical assessment, and reporting of potential site-related PFAS risks.

CERCLA Baseline Human Health Risk Assessment and Screening Level Ecological Risk Assessment for PFAS, Former March Air Reserve Base and Air Force Base, Riverside, California. Serves as principal in charge and technical lead for the PFAS baseline human health and ecological screening level risk assessment at the former installation. Supports the USAF and state agency discussions, development of risk assessment work plan with preliminary conceptual site model, selection of toxicity values, and exposure pathways and parameters for risk characterization.

CERCLA Baseline Human Health Risk Assessment and Screening Level Ecological Risk Assessment for PFAS, Mather Air Force Base, Sacramento County. Serves as principal in charge and technical lead for the PFAS baseline human health and ecological screening level risk assessment at the former installation. Supports the USAF and state agency discussions, development of risk assessment work plan with preliminary conceptual site model, selection of toxicity values, and exposure pathways and parameters for risk characterization.

1,4-Dioxane Site-Specific Risk Assessment and Consulting Support Related to Public Drinking Water System Contamination, Confidential Location. Provides risk assessment and technical support related to the regulatory basis and public health impacts of 1,4-dioxane in a public drinking water system.

EPA Toxic Substances and Control Act, Low Volume Exemption Application, Confidential Client. Provided human health toxicology and exposure assessment to support a low volume exemption (LVE) application to EPA TSCA program. Conduct analysis, develop report, and assist with in-person presentation to EPA TSCA technical staff.

Environmental Risk Assessment Oversight, U.S. Air Force Civil Engineering Center, Lackland, Texas. Provided toxicology expertise and oversight of risk assessments conducted for the USAF Environmental Restoration Program's CERCLA and RCRA activities. Using EPA's risk assessment guidance, interpreted toxicology data to assess risks to human health and the environment, and reviewed site-specific risk assessments conducted at USAF installations nationwide.

Environmental Justice

EPA Grant Environmental Justice Consulting, Keweenaw Bay Indian Community, Michigan. Provide human health toxicology and exposure assessment, and public training and science communication, to support the tribal community.

PUBLICATIONS ***(J.K. Anderson also Published as J.K. Hess-Wilson)***

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Selected Presentations and Posters (full list available upon request)

Anderson, J.K. 2024. U.S. Environmental Protection Agency, Toxic Substances Control Act PFAS Workshop: State-of-the-science and data gaps associated with fluoropolymers. Invited Speaker. February 13.

Anderson, J.K. 2023. 91st Annual Meeting of the United States Conference of Mayors – PFAS Human Health Risk: What Are the Potential Community Impacts to Low Levels. Columbus, OH. June 3.

Anderson, J.K. 2023. The Dallas Bar Association, Environmental Law CLE Program. The PFAS Circus – Science, Regulations, Legal Implications. March 23. Webinar

Anderson, J.K. 2023. National Turkey Federation Annual Meeting, Technical and Regulatory Committee Session. What's Your Proximity to the PFAS Problem? Palm Springs, CA. February 25.

Anderson, J.K. 2022. National Groundwater Association, PFAS Conference – PFAS and the Toxicological Challenges it (sic) Presents; PFAS Toxicology Overview and Challenges. June 22. Webinar

Anderson, J.K. 2022. US Conference of Mayors, 90th Annual Meeting. PFAS Regulatory Overview and Challenges. June 3. Panel Presentation

Anderson, J.K. 2022 NEWMOA, The Science of PFAS Conference. Overview of Site-specific Baseline Risk Assessments: What Are the Key Variables & Uncertainties for Characterizing PFAS Risk to Receptors. April 5. Presentation

Anderson, J.K. 2022. ERIS Webinar. Distilling the Facts from Fiction: How to Identify and Manage PFAS Risks in CRE Transactions. PFAS Toxicology and Regulatory Overview. February 8. Webinar

Whitehead K, J.K. Anderson, J. Skaggs, P. Williams. 2021. Microplastics as Emerging Contaminants. Austin Bar Association. October. Webinar

Anderson, J.K. 2021. National Groundwater Association, PFAS State of the Science. June. Webinar

Anderson, J.K. and L. Dell. 2021. PFAS Experts Symposium 2, Remediation Journal. Toxicology and Risk Assessment Committee: Human Health Effects. June 29. Webinar

Anderson, J.K. 2021. PFAS: State of the Science: Health, Human Exposure and Toxicological Aspects. National Groundwater Association, Fate of PFAS: From Groundwater to Tap Water Conference. June 22. Webinar

Anderson, J.K. 2021. PFAS Regulations Under the New Administration. Dallas Bar Association. May 27, 2021. Webinar

Anderson, J.K. 2021. 1,4-Dioxane: Science, Characterization & Analysis, and Remediation; Regulatory Framework, and Toxicology and Risk Assessment Modules. EPA CLU-IN Training. Live March 10. Available online: https://clu-in.org/conf/itrc/14D-1/

Anderson, J.K. 2020. PFAS the "Forever Chemical" that May Be Impacting Your Operations. AFS 32nd Environmental, Health and Safety Conference. October 6. Webinar.

Anderson, J.K., and P. Goodrum. 2019. PFAS: Toxicology and Regulatory Actions. Webinar to the ACC Public Health Advisory Board. November 7, 2019

Luz, A., C. Hutchings, J. Anderson, P. Goodrum, J. Field. 2019. A Novel Approach for Assessing Hazard Associated with Firefighting Foams. Poster at the SETAC North American 40th Annual Meeting, Toronto Ontario, Canada. November 4.

Anderson, J.K. 2019. Federal and State Environmental Guidance/Policies that Impact Remedial Decisions for PFAS. Platform presentation at the Washington State Advanced Superfund Conference. September 12, Seattle, WA.

Anderson, J.K. 2019. PFAS: Risk Characterization Panel. Invited panelist to the Society of Environmental Toxicology and Chemistry North America, Focused Technical Meeting on PFAS. Durham, NC. August.

Anderson, J.K., A. Luz, and P. Goodrum. 2019. Chronic human health toxicity value for perfluorohexanoate (PFHxA) and risk assessment relevant to current fluorotelomer-based chemistries. Poster for the Society of Toxicology 58th Meeting and ToxExpo, March 10–14, Baltimore, MD.

Goodrum, P., J.K. Anderson, and A. Luz. 2019. Perfluoroalkyl acid mixtures—Data analysis steps to uncover clues hidden in biomonitoring data. Poster for the Society of Toxicology 58th Meeting and ToxExpo, March 10–14, Baltimore, MD.

Luz, A., J.K. Anderson, and P. Goodrum. 2019. Approaches for Assessing Perfluoroalkyl Acid Mixture Toxicity. Poster for the Society of Toxicology 58th Meeting and ToxExpo, March 10–14, Baltimore, MD.

Opdyke, D., J. Benaman, J.K. Anderson, and J. Durda. 2019. An introduction to PFAS at contaminated sediment sites: Scientific and regulatory overview. Short course at Tenth International Conference on the Remediation and Management of Contaminated Sediments, February 11–14, New Orleans, LA.

Wilhelm, J., J.K. Anderson, A. Luz, and P. Goodrum. 2018. PFAAs and ecorisk: Development of a hazard ranking system by evaluating functional groups vs. chain lengths as primary risk drivers for ecological receptors. Poster presentation. SETAC North American 39th Annual Meeting, November 4–7, Sacramento, CA.

Luz, A.L., L. Tolbert, J.K. Anderson, P. Goodrum, D. Farrar, and S. Korzeniowski. 2018. PFHxA human health risks, margin of safety, and comparison with PFOA. Platform presentation. Society of Environmental Toxicology and Chemistry North America 39th Annual Meeting. November 4–8. Sacramento, CA.

Anderson, J.K. 2018. Emerging contaminants—per-and polyfluoroalkyl substances: A case study. Invited speaker. Texas Environmental Superconference, August, Austin, TX.

Anderson, J.K., and P. Goodrum. 2018. Internal and external dosimetry—the holy grail to decoding perfluoroalkyl acid toxicity? Poster presented at the Emerging Contaminants Summit, March 6–7, Westminster, CO.

Anderson, J.K., and P. Goodrum. 2018. What does that blood level mean? The assumptions underlying interpretations of health effects from internal doses. Poster presented at the Society of Toxicology 57th Annual Meeting and ToxExpo, March 11–15, San Antonio, TX.

Goodrum, P., and J.K. Anderson. 2018. Application of internal dosimetry for perfluoroalkyl acids and methods to assess uncertainty factors used in risk assessment. Poster presented at the Society of Toxicology 57th Annual Meeting and ToxExpo, March 11–15, San Antonio, TX.

Anderson, J.K. 2017. Uncertainty in the science of toxicology and emerging contaminants. Remediation of Emerging Contaminants: Trends in Science and Regulations. Montclair State University Continuing Education Course. June.

Anderson, J.K. 2017. Why the inconsistent and dynamic state and federal chemical regulatory landscape. RTM Communications Conference, Philadelphia, PA. April.

Anderson, J.K. 2016. Inconsistent and dynamic state and federal chemical regulations: Roadmap to success. Consumer Specialty Product Association annual conference. December.

Anderson, J.K. 2016. How did we get here from there? State and Federal regulatory actions for PFAS. AEHS Annual East Coast Conference. October.

Frankel, A., P.E. Goodrum, J.K. Anderson, and K. Tsitonaki. 2016. Water quality standards for perfluoroalkyl compounds—Crossroads between regulatory toxicology and remedy selection. Platform presentation, Battelle 10th International Conference on Remediation of Chlorinated and Recalcitrant Compounds, Palm Springs, CA.

Anderson, J.K., N. Edlin, and S. Herman. 2016. Keeping a watchful eye on emerging contaminants. Environmental and Emerging Claim Managers Association annual conference. April.

Anderson, J.K. 2016. Emerging contaminants: analytical, toxicity, regulatory, and legal frontiers. Invited panelist to the Emerging Contaminants Summit. March.

Anderson, J.K., and P.E. Goodrum. 2016. Emerging contaminants: crossroads of uncertain science and risk management. Integral Webinar Series. February.

Anderson, J.K., and P.E. Goodrum. 2015. Status of regulatory decisions for perfluoroalkyl compounds: is the level of protection to the general public worth the uncertainty and cost? Poster presented at Society for Risk Analysis, Washington, DC.

Anderson, J.K. 2015. Overview of regulatory toxicology in the development of federal and state MCLs for perfluoroalkyl compounds. AEHS Annual East Coast Conference. October.

PROFESSIONAL BACKGROUND

Principal, GSI Environmental Inc., Houston, Texas, 2020 – current

Senior Associate, GSI Environmental Inc., Houston, Texas, 2019

Senior Consultant, Integral Consulting Inc., San Antonio, Texas, 2015 – 2019

Emerging Issues and Contaminants Program Manager, Subject Matter Specialist – Toxicology, US Air Force Civil Engineer Center, San Antonio, Texas, 2010 – 2015

Post-Doctoral Fellow, National Center for Environmental Assessment, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, Ohio, 2007 - 2010

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS)

1 Introduction

The following topics are covered in this fact sheet:

- Polymer vs. Nonpolymer PFAS
- Perfluoroalkyl substances
- Polyfluoroalkyl substances
- PFAA Naming Conventions
- Long-Chain vs. Short-Chain
- Linear vs. Branched
- Acid vs. Anion
- Replacement Chemistry
- Physical and Chemical Properties

ITRC has developed a series of six fact sheets to summarize the latest science and emerging technologies regarding PFAS. The purpose of this fact sheet is to:

- Provide an overview of terminology, names, and acronyms for PFAS, focusing on those most commonly reported in the environment. The fact sheet focuses on those PFAS most commonly tested for by current analytical methods, but also describes other important classes of PFAS.
- Summarize the common physical and chemical properties associated with PFAS, along with a discussion of those properties for which no data are currently available.

For further information, please see the ITRC Technical and Regulatory Guidance document for PFAS dated April 2020.

This fact sheet uses three conventions worth highlighting:

- **Anionic form of chemical names:** Many PFAS can exist in various ionic states (for example, acids, anions, cations), which has important implications for their chemical and physical properties. In most cases, this fact sheet uses the anionic form of a given PFAS name, as this is the state in which most PFAS exist in the environment.
- **"PFC" is not used:** The acronym "PFC" is poorly defined in the scientific literature, but typically refers to "**per**fluorinated compounds." It does not include polyfluorinated substances which are increasingly recognized as important contaminants at many PFAS sites, while it does include unrelated chemicals that are not of concern at those sites.
- **"PFAS", not "PFASs":** The acronym "PFAS" stands for "per- **and** polyfluoroalkyl substances." No single chemical within the PFAS class can be both polyfluorinated and perfluorinated, so by definition "PFAS" is plural and a small "s" is not needed. Some authors elect to add a small "s" to this acronym (PFASs) to emphasize the fact that it is plural, but it is not needed. When referring to a single chemical within the PFAS class, it is usually more accurate to simply name that specific chemical.

USEPA has compiled an online resource for PFAS information. The information includes topics such as Policy and Guidance, Chemistry and Behavior, Occurrence, Toxicology, Site Characterization and Remediation Technologies (USEPA 2017h).

1.1 Why do we need to understand PFAS Naming Conventions?

The number and complexity of environmentally-relevant PFAS and the exponential increase in related scientific publications have led to confusion in the environmental community and the public (Buck et al. 2011; Wang et al. 2017). The use of non-specific acronyms, such as perfluorinated compound (PFC), has hampered clarity of investigative results. Use of consistent naming conventions by researchers, practitioners, regulators, and stakeholders will reduce confusion and support clearer communication.

Proper naming also helps to distinguish PFAS from other organic compounds that contain fluorine. PFAS, which are fluorinated aliphatic (carbon chain) substances, do not include aromatic (carbon ring) substances that contain carbon-fluorine (C-F) bonds (for example, active pharmaceutical ingredients, crop protection) or chlorofluorocarbons (refrigerants). This is another reason to avoid the use of the more generic acronym, PFC, which can include these non-PFAS.

Chemical Abstract Service (CAS) numbers are another helpful tool for clearly identifying the chemical that is being referenced. However, even these have led to confusion when it comes to PFAS. Some PFAS may occur in various ionic states, such as acids, anions (negatively charged), cations (positively charged salts), and zwitterions (both positively and negatively charged dipolar molecules), each of which has its own CAS number (and some have no CAS number). The ionic state determines its electrical charge and its physical and chemical properties, which in turn controls its fate and

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transport in the environment and potential human health and ecological effects. Chemical and physical properties of the various states of a given per- or polyfluoroalkyl substance can be so different that they completely alter critical aspects of the substance, such as solubility, volatility, and bioaccumulative potential. As a result, care must be taken in selecting the correct CAS number to avoid confusion regarding the chemistry and behavior of the chemical being described.

2 PFAS Families

PFAS encompass a wide universe of substances with very different physical and chemical properties, including gases (for example, perfluorobutane), liquids (for example, fluorotelomer alcohols), surfactants (for example, perfluorooctane sulfonate), and solid material high-molecular weight polymers (for example, polytetrafluoroethylene [PTFE]). For this reason, it is helpful to arrange PFAS that share similar chemical and physical properties into families.

The PFAS families may be divided into two primary categories: polymer and nonpolymer as shown in Figure 2-1. This fact sheet focuses primarily on nonpolymer PFAS most commonly detected in the environment. The polymer family of PFAS is not addressed in detail in this fact sheet. Buck et al. (2011) is an open-access paper that provides a more detailed explanation of PFAS terminology, classification, and origins, and recommends specific and descriptive terminology, names, and acronyms for PFAS.

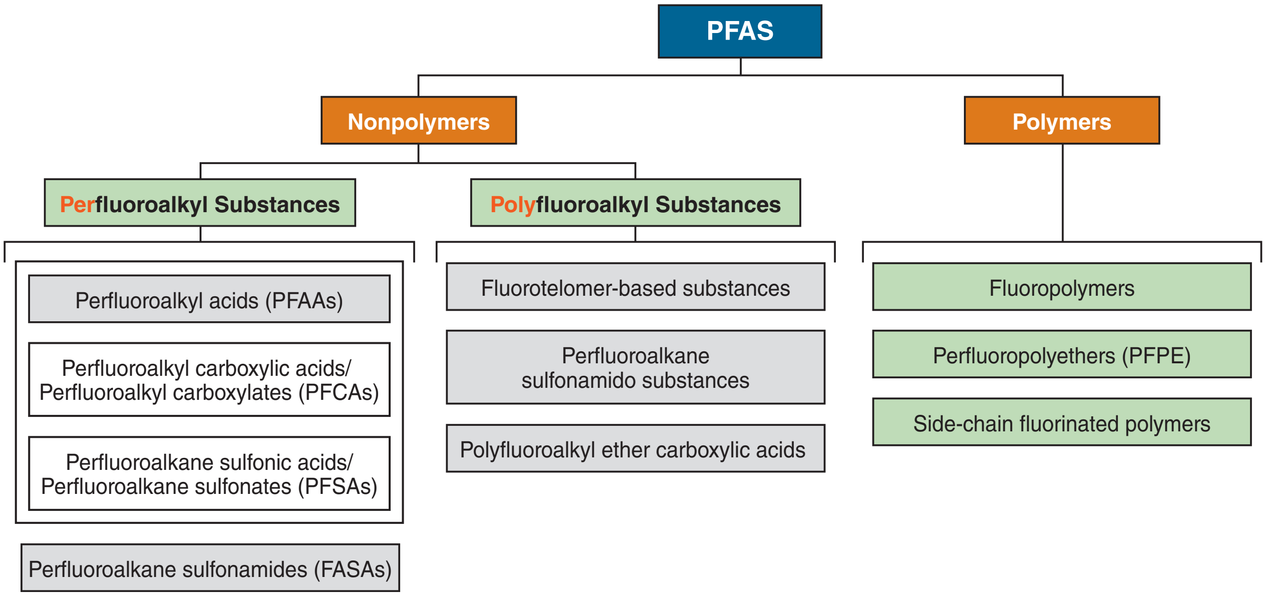


Figure 2-1. Summary of PFAS families

2.1 Nonpolymer PFAS

The family of nonpolymeric PFAS encompasses two major classes: perfluoroalkyl substances and polyfluoroalkyl substances, which include many subgroups of chemicals, examples of which are shown in Figure 2-1. Table 2-1 provides general classification and chemical structures, examples of each class, and primary uses of the nonpolymer PFAS highlighted in Figure 2-1. These compounds were selected as the focus of this fact sheet because they (1) are most commonly detected in humans, biota, and other environmental media; (2) appear to be relatively more abundant at PFAS investigation sites; (3) may have state or federal guidance values (see the *Regulations, Guidance, and Advisories Fact Sheet*); and/or (4) are included in most laboratory PFAS analyte lists.

2.1.1 Perfluoroalkyl Substances

Perfluoroalkyl substances are fully fluorinated (perfluoro-) alkane (carbon-chain) molecules. Their basic chemical structure is a chain (*or tail*) of two or more carbon atoms with a charged functional group *head* attached at one end. The functional groups commonly are carboxylates or sulfonates, but other forms are also detected in the environment. Fluorine atoms are attached to all possible bonding sites along the carbon chain of the tail, except for one bonding site on the last carbon where the functional group head is attached. This structure, which is illustrated in Figure 2-2 for perfluorooctane sulfonate (PFOS) and perfluorooctanoate (PFOA), can be written as:

$$\mathbf{C_nF_{2n+1}\text{-}R}$$

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

where "C_nF_{2n+1}" defines the length of the perfluoroalkyl chain tail, "n" is >2, and "R" represents the attached functional group head. Note that the functional group may contain 1 or more carbon atoms, which are included in the total number of carbons when naming the compound.

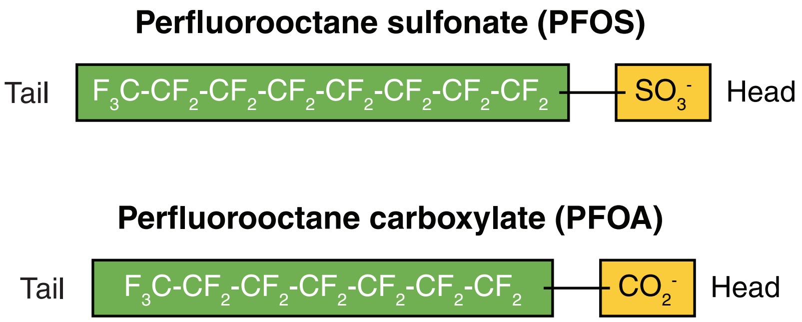


Figure 2-2. The tail and head structure of PFOS and PFOA molecules

Table 2-1. Major PFAS classes discussed in this fact sheet

Source: Adapted with permission from Buck, R.C., J. Franklin, U. Berger, J. M. Conder, I. T. Cousins, P. de Voogt, A. A. Jensen, K. Kannan, S. A. Mabury, and S. P. van Leeuwenet. 2011. "Perfluoroalkyl and Polyfluoroalkyl Substances in the Environment: Terminology, Classification, and Origins." Integrated Environmental Assessment and Management, 7:513-541. Open access. Copyright 2011 SETAC. http://dx.doi.org/10.1002/ieam.258

Family	Class	Group	General Chemical Structure: $C_nF_{2n+1}R$, where R =	Examples	Uses
PERFLUORINATED	Perfluoroalkyl acids (PFAAs)	Perfluoroalkyl carboxylic acids (PFCAs)	$-COOH$	Perfluorooctanoic acid (PFOA), $C_7F_{15}COOH$	Surfactant
		Perfluoroalkyl carboxylates (PFCAs)	$-COO^-$	Perfluorooctanoate (PFOA), $C_7F_{15}COO^-$	
		Perfluoroalkane sulfonic acids (PFSAs)	$-SO_3H$	Perfluorooctane sulfonic acid (PFOS), $C_8F_{17}SO_3H$	Surfactant
		Perfluoroalkane sulfonates (PFSAs)	$-SO_3^-$	Perfluorooctane sulfonate (PFOS), $C_8F_{17}SO_3^-$	
	Perfluoroalkane sulfonamides (FASAs)	Perfluoroalkane sulfonamides (FASAs)	$-SO_2NH_2$	Perfluorooctane sulfonamide (FOSA), $C_8F_{17}SO_2NH_2$	Major raw material for surfactant and surface protection products

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

Family	Class	Group	General Chemical Structure: $C_nF_{2n+1}R$, where R =	Examples	Uses
POLYFLUORINATED	Fluorotelomer substances	n:2 Fluorotelomer alcohols (n:2 FTOHs)	$-CH_2CH_2OH$	10:2 Fluorotelomer alcohol (10:2 FTOH), $C_{10}F_{21}CH_2CH_2OH$	Major raw material for surfactant and surface protection products
		n:2 Fluorotelomer sulfonic acids (n:2 FTSAs)	$-CH_2CH_2SO_3H$	8:2 Fluorotelomer sulfonic acid (8:2 FTSA), $C_8F_{17}CH_2CH_2SO_3H$	Surfactant and environmental transformation products
		Fluorotelomer carboxylic acids (FTCAs)	$-CH_2COOH$	6:2 Fluorotelomer carboxylic acid (6:2 FTCA), $C_6F_{13}CH_2COOH$	Intermediate environmental transformation product
			$-CH_2CH_2COOH$	5:3 Fluorotelomer carboxylic acid (5:3 Acid), $C_5F_{11}CH_2CH_2COOH$	
	Perfluoroalkane sulfonamido substances	N-alkyl perfluoroalkane sulfonamides (N-alkyl FASAs) (MeFASAs, EtFASAs, BuFASAs)	$-SO_2N(R')H$ where $R' = C_mH_{2m+1}$ (m = 1, 2,4)	N-Ethyl perfluorooctane sulfonamide (EtFOSA), $C_8F_{17}SO_2N(C_2H_5)H$	Major raw material for surfactant and surface protection products
				N-Methyl perfluorooctane sulfonamide (MeFOSA), $C_8F_{17}SO_2N(CH_3)H$	
		Perfluoroalkane sulfonamido ethanols (FASEs) and N-alkyl perfluoroalkane sulfonamido ethanols (MeFASEs, EtFASEs, BuFASEs)	$SO_2N(R')CH_2CH_2OH$ where $R' = C_mH_{2m+1}$ (m = 0, 1, 2, 4)	N-Ethyl perfluorooctane sulfonamidoethanol (EtFOSE), $C_8F_{17}SO_2N(C_2H_5)CH_2CH_2OH$	Major raw material for surfactant and surface protection products
				N-Methyl perfluorooctane sulfonamido ethanol (MeFOSE), $C_8F_{17}SO_2N(CH_3)CH_2CH_2OH$	
		Perfluoroalkane sulfonamido acetic acids (FASAAs) and N-alkyl perfluoroalkane sulfonamido acetic acids (MeFASAAs, EtFASAAs, BuFASAAs)	$SO_2N(R')CH_2COOH$ where $R' = C_mH_{2m+1}$ (m = 0, 1, 2,4)	N-Ethyl perfluorooctane sulfonamido acetic acid (EtFOSAA), $C_8F_{17}SO_2N(C_2H_5)CH_2CO_2H$	Intermediate environmental transformation product
				N-Methyl perfluorooctane sulfonamido acetic acid (MeFOSAA), $C_8F_{17}SO_2N(CH_3)CH_2CO_2H$	

2.1.1.1 Perfluoroalkyl acids (PFAAs)

Perfluoroalkyl acids (PFAAs) are some of the most basic PFAS molecules. They are essentially non-degradable and currently are the class of PFAS most commonly tested for in the environment. Biotic and abiotic degradation of many polyfluoroalkyl substances may result in the formation of PFAAs. As a result, PFAAs are sometimes referred to as "terminal PFAS" or "terminal degradation products," meaning no further degradation products will form from them under environmental conditions. Polyfluoroalkyl substances that degrade to create terminal PFAAs are referred to as "precursors." The PFAA class is divided into two major groups (also shown in Table 2-1):

- *Perfluoroalkyl carboxylic acids* (PFCAs), or perfluoroalkyl carboxylates, are terminal degradation products of select precursor polyfluoroalkyl substances, such as fluorotelomer alcohols (FTOHs). The most frequently detected PFCA is PFOA.
- *Perfluoroalkane sulfonic acids* (PFSAs), or perfluoroalkyl sulfonates, are also terminal degradation products of select precursor polyfluoroalkyl substances, such as perfluoroalkyl sulfonamidoethanols (FASEs). The most frequently detected PFSA is PFOS.

2.1.1.2 Perfluoroalkane sulfonamides (FASAs)

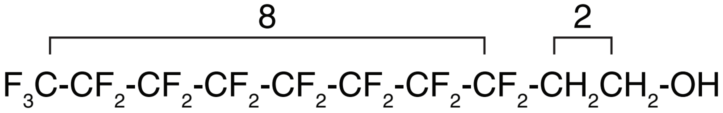
Perfluoroalkane sulfonamides (FASAs), such as perfluorooctane sulfonamide (FOSA), are used as raw material to make perfluoroalkyl sulfonamide substances that are used for surfactants and surface treatments. FASAs can degrade to form PFAAs such as PFOS.

2.1.2 Polyfluoroalkyl Substances

Polyfluoroalkyl substances and some side-chain fluorinated polymers are increasingly being identified as important to understanding the fate and transport of PFAS at release sites and in the environment (OECD 2013; Butt, Muir, and Mabury 2014; Liu and Mejia-Avendaño 2013; Wang et al. 2011; Mejia-Avendaño et al. 2016). Figure 2-1 highlights the polyfluoroalkyl substances that, to date, have most commonly been detected at PFAS sites (see Barzen-Hanson et al. 2017).

Polyfluoroalkyl substances are distinguished from perfluoroalkyl substances by not being fully fluorinated. Instead, they have a non-fluorine atom (typically hydrogen or oxygen) attached to at least one, but not all, carbon atoms, while at least two or more of the remaining carbon atoms in the carbon chain tail are fully fluorinated (Figure 2-3).

Fluorotelomer-based polyfluoroalkyl substances are named using an "n:x" prefix where "n" indicates the number of fully fluorinated carbon atoms (n >2) and "x" indicates the number of carbon atoms that are not fully fluorinated (x > 1). An example of a polyfluoroalkyl substance is shown in Figure 2-3, which also illustrates the "n:x" naming convention.



$$\overbrace{F_3C\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2}^{8}\text{-}\overbrace{CH_2CH_2}^{2}\text{-}OH$$

8:2 FTOH (8:2 fluorotelomer alcohol)

Figure 2-3. Example of a polyfluoroalkyl substance where two of the carbons in the tail are not fully fluorinated, while the remaining carbons are. This also illustrates the "n:x" naming convention where "n" is the number of fully fluorinated carbons (in this case, 8) and "x" is the number of carbons that are not fully fluorinated (in this case, 2).

The carbon-hydrogen (or other non-fluorinated) bond in polyfluoroalkyl molecules creates a "weak" point in the carbon chain that is susceptible to biotic or abiotic degradation. As a result, many polyfluoroalkyl substances that contain a perfluoroalkyl C_nF_{2n+1} group are potential precursor compounds that have the potential to be transformed into PFAAs.

Figures 2-4 and 2-5 provide some examples of degradation pathways for environmentally relevant polyfluoroalkyl precursors derived from two PFAS production methods, telomerization and electrochemical fluorination (ECF), respectively. Note that these figures include some PFAS not discussed in this fact sheet, but described in Buck et al. (2011).

2.1.2.1 Fluorotelomer Substances

Fluorotelomer substances are polyfluoroalkyl substances produced by the fluorotelomerization process. As shown in Figure 2-4, the degradation of fluorotelomer-based substances is a potential source of PFCAs in the environment, but not PFSAs (Buck et al. 2011). For many of these compounds, the naming convention identifies the number of fully fluorinated carbon atoms and the number of carbon atoms that are not fully fluorinated.

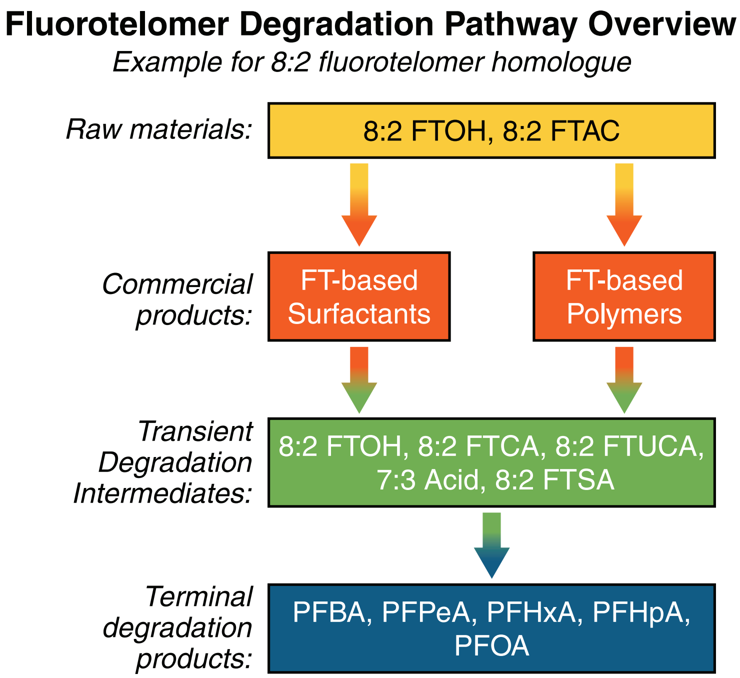


Figure 2-4. Fluorotelomer degradation pathway overview (*Example for 8:2 fluorotelomer homologue*)

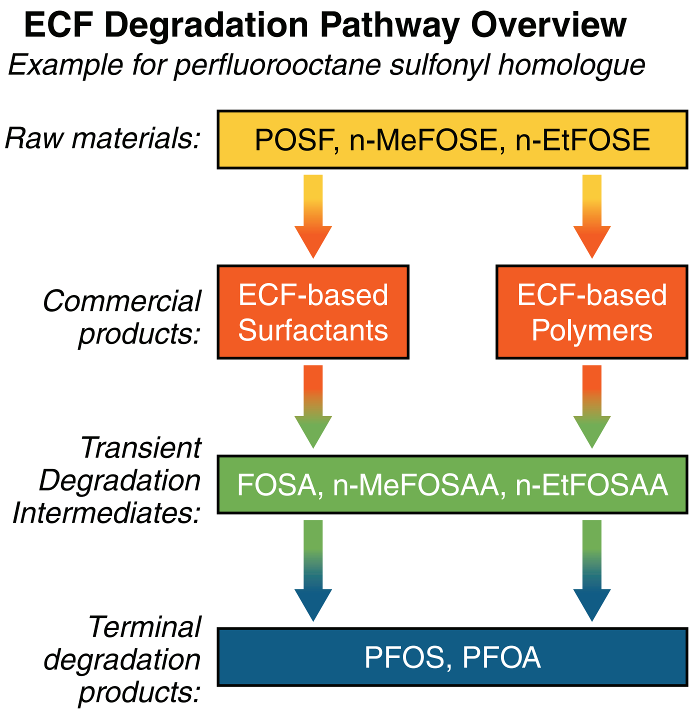


Figure 2-5. ECF degradation pathway overview (*Example for perfluorooctane sulfonyl homologue*).

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

The following fluorotelomer substances (also shown in Table 2-1) are those most commonly detected in the environment to date:

- *Fluorotelomer alcohols* (FTOH): The n:2 fluorotelomer alcohols (n:2 FTOHs) are key raw materials in the production of n:2 fluorotelomer acrylates and n:2 fluorotelomer methacrylates (Buck et al. 2011).
- *Fluorotelomer sulfonic acids* (FTSA): The n:2 fluorotelomer sulfonic acids (n:2 FTSAs) have been detected in environmental matrices at sites where aqueous film forming foam (AFFF) has been used, and also in wastewater treatment plant effluents and landfill leachate. FTSAs are precursor compounds and can undergo aerobic biotransformation to form PFCAs (Buck et al. 2011).
- *Fluorotelomer carboxylic acids* (FTCA): These compounds form through the biodegradation of FTOHs (Figure 2-3; Buck et al. 2011; Liu and Mejia Avendaño 2013) and have been detected in landfill leachate. Note that the –COOH functional group on these fluorotelomer compounds mean they may have either an even or odd number of carbons, so they may have n:2 or n:3 prefixes.

2.1.2.2 Perfluoroalkane Sulfonamido Substances

All of the families of perfluoroalkane sulfonamido substances shown in Table 2-1 and discussed below have been detected in the environment and humans. *Perfluoroalkane* refers to the fully fluorinated carbon chain tail, but these compounds also contain one or more CH2 groups in the head of the molecule attached to the sulfonamido spacer (see Figure 2-6). They are either used as raw materials for surfactant and surface treatment products, or they are present as intermediate transformation products of these raw materials. As shown in Figure 2-5, some perfluoroalkane sulfonamido substances have been found to degrade to PFOS (Mejia Avendaño and Liu 2015). Environmentally relevant perfluoroalkane sulfonamido substances include:

- *Perfluoroalkane sulfonamido ethanols* (FASEs) and *N-alkyl perfluoroalkane sulfonamido ethanols* (MeFASEs, EtFASEs, BuFASEs) are raw materials for surfactant and surface treatment products (Buck et al. 2011). Figure 2-6 illustrates the structure of N-EtFOSE.
- *Perfluoroalkane sulfonamido acetic acids* (FASAAs) and *N-alkyl perfluoroalkane sulfonamido acetic acids* (MeFASAAs, EtFASAAs, BuFASAAs) are intermediate transformation products of FASEs, MeFASEs, EtFASEs, and BuFASEs (see Figure 2-5) (Buck et al. 2011).
- *N-alkyl perfluoroalkane sulfonamides (N-alkyl FASAs)* are transformation rpoducts that include N-Methyl perfluorooctane sulfonamide (MeFOSA) and N-Ethyl perfluorooctane sulfonamide (EtFOSA).

NEtFOSE (n-ethyl perfluorooctane sulfonamido ethanol)

Figure 2-6. Example perfluoroalkane sulfonamido ethanol (FASE)

2.2 Polymer PFAS

Polymers are large molecules formed by combining many identical smaller molecules (or monomers) in a repeating pattern. Polymer substances in the PFAS family include fluoropolymers, perfluoropolyethers (PFPE), and side-chain fluorinated polymers.

Side-chain fluorinated polymers contain a nonfluorinated polymer backbone from which fluorinated side chains branch off. Some may become precursors for PFAAs when the point of connection of a fluorinated side-chain on a polymer is broken to release a PFAA.

In general, some polymer PFAS are currently believed to pose less immediate human health and ecological risk relative to some nonpolymer PFAS. As stated previously, most compounds of interest at environmental release sites are nonpolymers.

3 PFAA Naming Conventions

PFAAs are the group of PFAS that make up the majority of PFAS typically included in commercial laboratory target analyte lists and are the primary PFAS for which federal or state health-based guidance values have been established. As a result, they tend to drive site investigation and remediation decisions, and so it is helpful to understand the naming conventions for this class. Many of the commonly detected PFAAs are denoted using the structural shorthand:

PFXY

where:
PF = perfluoroalkyl
X = the carbon chain length (using the same naming conventions as hydrocarbons based on the number of carbons ([for example, B for butane or 4 carbons, Pe for pentane or 5 carbons])
Y = the functional group

Table 3-1 illustrates how this naming structure works for the PFCAs and PFSAs, which collectively are referred to as PFAAs.

Table 3-1. Basic naming structure and shorthand for perfluoroalkyl acids (PFAAs)

X	Y	Acronym	Name	Formula	CAS No.
B = buta (4 carbon)	A = Carboxylate or carboxylic acid	PFBA	Perfluorobutanoate	$C_3F_7CO_2^-$	45048-62-2
			Perfluorobutanoic acid	C_3F_7COOH	375-22-4
	S = Sulfonate or sulfonic acid	PFBS	Perfluorobutane sulfonate	$C_4F_9SO_3^-$	45187-15-3
			Perfluorobutane sulfonic acid	$C_4F_9SO_3H$	375-73-5
Pe = penta (5 carbon)	A = Carboxylate or carboxylic acid	PFPeA	Perfluoropentanoate	$C_4F_9CO_2^-$	45167-47-3
			Perfluoropentanoic acid	C_4F_9COOH	2706-90-3
	S = Sulfonate or sulfonic acid	PFPeS	Perfluoropentane sulfonate	$C_5F_{11}SO_3^-$	175905-36-9
			Perfluoropentane sulfonic acid	$C_5F_{11}SO_3H$	2706-91-4
Hx = hexa (6 carbon)	A = Carboxylate or carboxylic acid	PFHxA	Perfluorohexanoate	$C_5F_{11}CO_2^-$	92612-52-7
			Perfluorohexanoic acid	$C_5F_{11}COOH$	307-24-4
	S = Sulfonate or sulfonic acid	PFHxS	Perfluorohexane sulfonate	$C_6F_{13}SO_3^-$	108427-53-8
			Perfluorohexane sulfonic acid	$C_6F_{13}SO_3H$	355-46-4
Hp = hepta (7 carbon)	A = Carboxylate or carboxylic acid	PFHpA	Perfluoroheptanoate	$C_6F_{13}CO_2^-$	120885-29-2
			Perfluoroheptanoic acid	$C_6F_{13}COOH$	375-85-9
	S = Sulfonate or sulfonic acid	PFHpS	Perfluoroheptane sulfonate	$C_7F_{15}SO_3^-$	146689-46-5
			Perfluoroheptane sulfonic acid	$C_7F_{15}SO_3H$	375-92-8
O = octa (8 carbon)	A = Carboxylate or carboxylic acid	PFOA	Perfluorooctanoate	$C_7F_{15}CO_2^-$	45285-51-6
			Perfluorooctanoic acid	$C_7F_{15}COOH$	335-67-1
	S = Sulfonate or sulfonic acid	PFOS	Perfluorooctane sulfonate	$C_8F_{17}SO_3^-$	45298-90-6
			Perfluorooctane sulfonic acid	$C_8F_{17}SO_3H$	1763-23-1
N = nona (9 carbon)	A = Carboxylate or carboxylic acid	PFNA	Perfluorononanoate	$C_8F_{17}CO_2^-$	72007-68-2
			Perfluorononanoic acid	$C_8F_{17}COOH$	375-95-1
	S = Sulfonate or sulfonic acid	PFNS	Perfluorononane sulfonate	$C_9F_{19}SO_3^-$	474511-07-4
			Perfluorononane sulfonic acid	$C_9F_{19}SO_3H$	68259-12-1
D = deca (10 carbon)	A = Carboxylate or carboxylic acid	PFDA	Perfluorodecanoate	$C_9F_{19}CO_2^-$	73829-36-4
			Perfluorodecanoic acid	$C_9F_{19}COOH$	335-76-2
	S = Sulfonate or sulfonic acid	PFDS	Perfluorodecane sulfonate	$C_{10}F_{21}SO_3^-$	126105-34-8
			Perfluorodecane sulfonic acid	$C_{10}F_{21}SO_3H$	335-77-3

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

X	Y	Acronym	Name	Formula	CAS No.
Un = undeca (11 carbon)	A = Carboxylate or carboxylic acid	PFUnA or PFUnDA	Perfluoroundecanoate	$C_{10}F_{21}CO_2^-$	196859-54-8
			Perfluoroundecanoic acid	$C_{10}F_{21}COOH$	2058-94-8
	S = Sulfonate or sulfonic acid	PFUnS or PFUnDS	Perfluoroundecane sulfonate	$C_{11}F_{23}SO_3^-$	441296-91-9
			Perfluoroundecane sulfonic acid	$C_{11}F_{23}SO_3H$	749786-16-1
DoD = dodeca (12 carbon)	A = Carboxylate or carboxylic acid	PFDoDA	Perfluorododecanoate	$C_{11}F_{23}CO_2^-$	171978-95-3
			Perfluorododecanoic acid	$C_{11}F_{23}COOH$	307-55-1
	S = Sulfonate or sulfonic acid	PFDoDS	Perfluorododecane sulfonate	$C_{12}F_{25}SO_3^-$	343629-43-6
			Perfluorododecane sulfonic acid	$C_{12}F_{25}SO_3H$	79780-39-5
TrD = trideca (13 carbon)	A = Carboxylate or carboxylic acid	PFTrDA	Perfluorotridecanoate	$C_{12}F_{25}CO_2^-$	862374-87-6
			Perfluorotridecanoic acid	$C_{12}F_{25}COOH$	72629-94-8
	S = Sulfonate or sulfonic acid	PFTrDS	Perfluorotridecane sulfonate	$C_{13}F_{27}SO_3^-$	NA
			Perfluorotridecane sulfonic acid	$C_{13}F_{27}SO_3H$	NA
TeD = tetradeca (14 carbon)	A = Carboxylate or carboxylic acid	PFTeDA	Perfluorotetradecanoate	$C_{13}F_{27}CO_2^-$	365971-87-5
			Perfluorotetradecanoic acid	$C_{13}F_{27}COOH$	376-06-7
	S = Sulfonate or sulfonic acid	PFTeDS	Perfluorotetradecane sulfonate	$C_{14}F_{29}SO_3^-$	NA
			Perfluorotetradecane sulfonic acid	$C_{14}F_{29}SO_3H$	NA

NA = not available

Note that for carboxylates, the total number of carbons used for naming the compound includes the carbon in the carboxylic acid functional group (COOH), and so although PFOA has seven carbons in its fluoroalkyl tail, all eight of the carbons in the molecule are used to name it, hence *perfluorooctanoate*. However, in terms of chemical behavior, PFOA would be more analogous to seven-carbon perfluoroheptane sulfonate, PFHpS, than to eight-carbon perfluorooctane sulfonate, PFOS.

Note that in Table 3-1, PFAA names and formulas are shown in both the anionic (also referred to as “deprotonated”) and acid (or neutral; also referred to as protonated) forms. The anionic form is the state that PFAAs are found in the environment, except in very rare situations (for example, extremely low pH). The anionic and acid forms of PFAA names are often incorrectly used interchangeably (for example, perfluorooctane sulfonate and perfluorooctane sulfonic acid), and the same acronym (in this case, PFOS) applies to both forms. However, as discussed in Sections 3.2 and 6.2.2, their physical and chemical properties are different and it is important to know which form is being described.

Until recently, carboxylates and sulfonates have been the classes most commonly tested for in the environment. However, a wide range of PFAS with other functional groups exist for which the same “PFXY” shorthand shown above may or may not apply. For naming conventions for these compounds, please refer to Buck et al. (2011).

A Note About PFAS Naming in Laboratory Reports

Even though PFAAs occur as anions in the environment, some laboratories report all of their results in the acidic form, while others may report PFCAs as acids (for example, perfluorooctanoic acid) and PFSAs as anions (for example, perfluorooctane sulfonate). Different naming conventions in laboratory reports has led to confusion regarding exactly which form of the PFAA they are measuring. Although the lab is measuring the concentration of PFAA anions present in the sample, where the results are reported as an acid, the lab has adjusted for the H^+ cation (which has so little mass, this does not affect the resulting concentration).

It should be noted that the standards used by laboratories to perform analyses may be prepared from PFAA salts, as is often the case for sulfonate standards. If so, the lab must adjust the reported concentration to account for the mass of the counterion (typically Na+ or K+). The calculation to do this is described in Section 7.2.3 of EPA Method 537 (Shoemaker, Grimmett, and Boutin 2009).

3.1 Long Chain versus Short Chain Distinction

PFAAs are sometimes described as *long-chain* and *short-chain* as a shorthand way to group PFCAs and PFSAs that may behave similarly in the environment. However, it is important not to make generalizations about PFAA behavior based only on chain length. As recent research suggests, other factors besides chain length may affect bioaccumulation potential of PFAS (Ng and Hungerbühler 2014).

According to the Organisation for Economic Co-operation and Development (OECD 2013):

- *Long-chain* refers to:
    - o perfluoroalkyl carboxylic acids, PFCAs, with eight or more carbons (seven or more carbons are perfluorinated)
    - o perfluoroalkane sulfonates, PFSAs, with six or more carbons (six or more carbons are perfluorinated)

- *Short-chain* refers to:
    - o perfluoroalkyl carboxylic acids with seven or fewer carbons (six or fewer carbons are perfluorinated)
    - o perfluoroalkane sulfonates with five or fewer carbons (five or fewer carbons are perfluorinated)

Table 3-2 illustrates the differences in the short-chain and long-chain PFCAs and PFSAs.

Table 3-2. Short-chain and long-chain PFCAs and PFSAs

Number of Carbons	4	5	6	7	8	9	10	11	12
PFCAs	Short-chain PFCAs				Long-chain PFCAs				
	PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDoA
PFSAs	PFBS	PFPeS	PFHxS	PFHpS	PFOS	PFNS	PFDS	PFUnS	PFDoS
	Short-chain PFSAs		Long-chain PFSAs						

3.2 Anion versus Acid Form

As noted above, the names for the anionic and acid forms of PFAAs are often used interchangeably. However, it is critical to know which form is being discussed because of differences in their physical and chemical properties and behavior in the environment (see Section 6). Some important things to keep in mind regarding the anionic vs. acid forms are:

- Most PFAAs are present in environmental and human matrices in their anionic form. For example, PFOS is present in the environment in the anionic form, perfluorooctane sulfonate.
- Although laboratories may be reporting PFOA or PFOS using the acid form of their name, they are actually measuring the anionic form (for example, octanoate or sulfonate), as this is the form that exists in the environment.
- The acid form and their associated cationic salts have CAS numbers, while the anionic forms may not (see Table 3-1). For example, PFOS can exist as different salts (cationic), including sodium, lithium, potassium, or ammonium. Each of these salts will have a different CAS number:
    - o PFOS, acid form CAS No.: 1763-23-1
    - o PFOS, potassium salt CAS No.: 2795-39-3
    - o PFOS, ammonium salt CAS No.: 29081-56-9
- When the salt or acid exists in water or other liquids, it will dissociate and the salt or acid will break off and form the anion (COO^-). Figure 3-1 illustrates the dissociation of perfluorobutanoic acid.
- It is most important to distinguish between the acid form and anionic form when reporting the physical and chemical properties. The discussion of PFAS properties in this fact sheet generally refers to the anionic form; it will be specifically called out if the acid form is being discussed.

$$F_3C\text{-}CF_2\text{-}CF_2\text{-}COOH \rightleftharpoons F_3C\text{-}CF_2\text{-}CF_2\text{-}CO_2^- + H^+$$

Perfluorobutanoic acid **Perfluorobutanoate (+ dissociated proton)**

Figure 3-1. Dissociation of perfluorobutanoic acid

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

4 Linear and Branched Isomers of PFAS

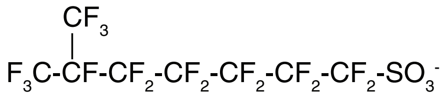
Many PFAS may be present as mixtures of linear and branched isomers (chemicals with the same chemical formula, but different molecular structures) depending on the manufacturing process that was used. These structural differences are important because they may affect how the compounds behave in the environment and may provide an indicator of their source. Structural differences are described below:

- A *linear isomer* is composed of carbon atoms bonded to only one or two carbons, which form a straight carbon backbone. There can be only one linear isomer in a C_n homologue (compounds with the same number of carbons in their tail) series.
- In a *branched isomer*, at least one carbon atom is bonded to more than two carbon atoms, which forms a branching of the carbon backbone. There can be many isomers per C_n homologue series.

Figure 4-1 illustrates the structures of linear and branched PFOS.

$F_3C\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}SO_3^-$

Linear Perfluorooctane sulfonate (PFOS)



$$F_3C\text{-}\overset{\overset{CF_3}{|}}{C}F\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}CF_2\text{-}SO_3^-$$

Branched Perfluorooctane sulfonate (PFOS)

Figure 4-1. Linear and one branched isomer of PFOS

The formula "C_nF_{2n+1}-" (where n is greater than or equal to 3) includes linear and branched structures. For example, PFOS and PFHxS are routinely present in environmental samples as a mixture of linear and branched isomers.

Accurate quantification of PFAS that are mixtures of linear isomers and branched isomers in environmental matrices can be difficult (Riddell et al. 2009). However, they may be useful in understanding sources of PFAS and the age of the source, since the production of isomers varies by manufacturing processes. For example, the fluorotelomerization process produces primarily linear PFAAs, whereas the ECF process produces a mixture of linear and branched PFAA isomers (see Table 4-1 and the *History and Use Fact Sheet*). The presence of linear and branched isomers may also have implications for partitioning and transport.

Table 4-1. Manufacturing processes and potential PFAAs produced

Manufacturing Process	Commonly Found Polyfluorinated Substance (Precursors)	Potential PFAAs Produced
Telomerization	FTSA[1]	Linear PFCAs
	FTCA[2]	Linear PFCAs
	FTOH	Linear PFCAs
Electrochemical Fluorination	FASE	Branched and Linear PFCAs Branched and Linear PFSAs
	FASAA	Branched and Linear PFCAs Branched and Linear PFSAs

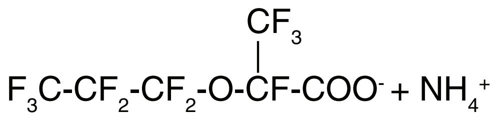
[1] Fluorotelomer sulfonate: found at AFFF sites
[2] Fluorotelomer carboxylic acids (for example, 5:3 Acid) found in landfill leachate

5 Replacement Chemistry

Concern regarding the persistence, bioaccumulation, and possible ecological and human health effects of long-chain PFAAs has led manufacturers to develop replacement short-chain PFAS chemistries that should not degrade to long-chain PFAAs (USEPA 2006a; OECD 2017). The short-chain alternatives include fluorotelomer-based products with a six-carbon perfluorohexyl chain and ECF-based products with a four-carbon perfluorobutyl chain. These products may degrade to form short-chain PFAAs, such as PFHxA and PFBS, respectively (Wang et al. 2013; Buck 2015). While a full discussion of such replacement chemistries is not possible here, it is important to be aware of this trend toward shorter-chain chemistries, as some of these PFAS increasingly may be detected in the environment.

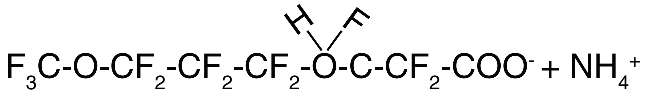
Examples of this trend are replacement PFAS that have been developed for use as processing aids in the manufacturing of fluoropolymers. The replacements are generally fluorinated ether carboxylates. Two of these that have been detected in the environment and generated public concern and regulatory actions are given here (their molecular structures are illustrated in Figure 5-1):

- GenX – trade name for ammonium, 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy) propanoate ($CF_3CF_2CF_2OCF(CF_3)COO^- NH_4^+$, CAS No. 62037-80-3), a perfluoropolyether carboxylate surfactant (Wang et al. 2013; Buck 2015)
- ADONA – trade name for ammonium 4,8-dioxa-3H-perfluorononanoate ($CF_3OCF_2CF_2CF_2\text{-}OCHFCF_2COO^-NH_4^+$ (CAS No. 958445-44-8), a polyfluoropolyether carboxylate surfactant (Gordon 2011)



$$F_3C\text{-}CF_2\text{-}CF_2\text{-}O\text{-}\overset{\overset{\displaystyle CF_3}{|}}{C}F\text{-}COO^- + NH_4^+$$

GenX



ADONA

Figure 5-1. Example replacement chemistry structures

6 Physical and Chemical Properties

The physical and chemical properties of PFAS, in concert with the characteristics of the environmental system, determine the environmental behavior of organic contaminants, including the compound's state and partitioning behavior (Banks, Smart, and Tatlow 1994). Partitioning can occur between neutral and ionic molecular forms, solid and liquid states, and between different media and biota (aqueous, pure phase, soil/sediment, biota, and atmospheric). The environmental behavior of many PFAS is further complicated by their surfactant properties.

Figure 6-1 illustrates key chemical and physical properties and distribution coefficients. Comparing the chemical and physical properties of different PFAS provides insight into similarities and differences in their environmental behavior and can inform investigation design.

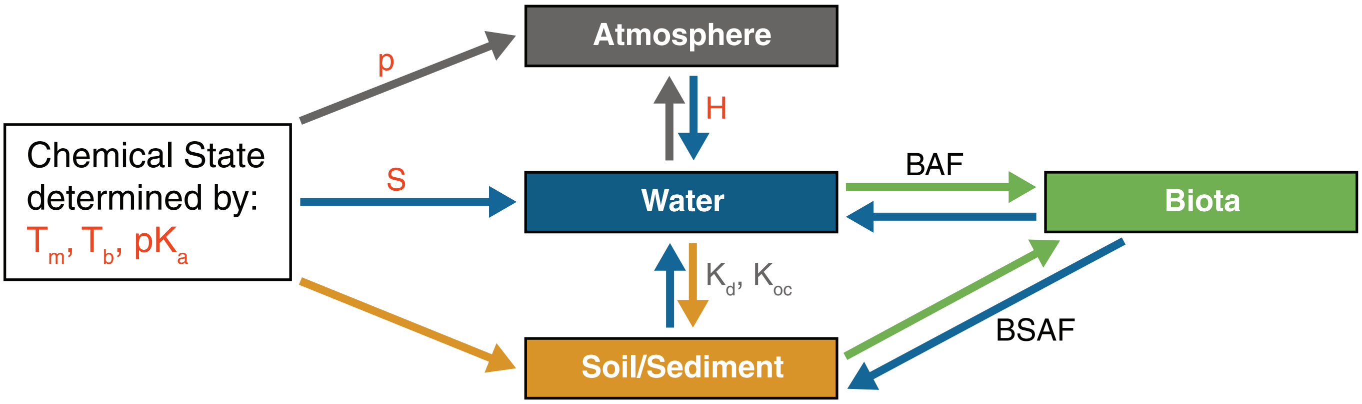


Figure 6-1. The role of key physical and chemical properties (shown in red) in influencing environmental compound behavior. Other key distribution coefficients (for example, Kd, Koc shown in grey) are addressed in the *Environmental Fate and Transport Fact Sheet*. Tm = melting point; Tb = boiling point; pKa = acid dissociation constant; p = vapor pressure; S = solubility; H = dimensionless Henry's law constant; Kd = soil and sediment partitioning coefficient; Koc = organic carbon partitioning coefficient; BAF = bioaccumulation factor; and BSAF = biota-sediment accumulation factor.

Naming Conventions and Physical and Chemical Properties of Per- and Polyfluoroalkyl Substances (PFAS) *continued*

There is a large variation in published data on chemical and physical properties of PFAS. Reliable physical and chemical properties of PFAS are scarce (for example, vapor pressure and Henry's law constants), and some of the available values are modeled, as opposed to directly measured. With a few exceptions (Koc and BCF or BAF values), many of the available properties are based on the acid form of the PFAA, which is not present in the environment, unless at pH <3, which is not typical. Table 6-1 provides a general summary of the available chemical and physical property information for PFCAs and the sensitivity of this information in relation to the acid vs. anionic form. For example, the anionic forms of PFOA and PFOS have documented bioconcentration factor and bioaccumulation factor properties (Martin et al. 2003a; 2003b) while other properties are not readily available.

Table 6-1. Available physical and chemical properties for PFCAs

Properties								Environmentally Relevant?
PFAA State	CAS No.	S_w	P^o	K_h	K_{ow}	K_{oc}	BCF and/or BAF	
Acid	Y	Y	Y	E	E	E	N	No
Cation:								No
NH_4^+	Y	Y	N	N	N	N	N	
Li^+	Y	Y	N	N	N	N	N	
Na^+	Y	Y	N	N	N	N	N	
Anion	M	N	N	N	N	Y	Y	Yes

S_w = solubility in water
P^o = vapor pressure
K_h = Henry's Law Constant
K_{ow} = octanol/water partition coefficient
K_{oc} = organic carbon partition coefficient
BAF = bioaccumulation factor
BCF = bioconcentration factor

Y = data available
N = no data available
M = data may be available for some
E = data estimated, not directly measured

6.1 Physical Properties

Many PFAS are in solid form at room temperature, often as a white powder or waxy substance, though some may be liquids. As mentioned before, data regarding physical properties of PFAS are scarce, and for PFAAs may relate to the acid form of the compound, which is not the most environmentally relevant form. Some melting point data are available for standards of PFCAs in the acid form. Measured vapor pressures for the acid form of PFOA, PFNA, PFDA, PFUnA, and PFDoA (Barton, Botelho, and Kaiser 2008; Kaiser et al. 2005) and fluorotelomer alcohols (Krusic et al. 2005) are also available. Similarly, Henry's Law constants are available for fluorotelomer alcohols (Goss et al. 2006). For PFAAs, the acid form is known to partition into air from aqueous solutions at very low pH (Kaiser et al. 2010). Care should be taken when reviewing available physical property information for PFAS to ensure that it applies to the form (for example, acid or anionic) of concern to the project or site in question.

6.2 Chemical Properties

6.2.1 Fluorine and the Carbon-fluorine (C-F) Bond

As previously mentioned, understanding PFAS chemical properties is key to understanding the diversity of uses and applications associated with this class of compounds, as well as their unique environmental behavior. Some key fluorine chemical properties and the characteristics they impart to PFAS are provided in Table 6-2.

Properties such as the high electronegativity and small size of fluorine lead to a strong C-F bond, the strongest covalent bond in organic chemistry (Kissa 2001; Banks, Smart, and Tatlow 1994). The low polarizability of fluorine further leads to weak intermolecular interactions, such as van der Waals interactions and hydrogen bonding (Kissa 2001; Banks, Smart, and Tatlow 1994). It is mainly the unique properties of fluorine that give many PFAS their mutually hydro- and lipophobic (stain-resistant) and surfactant properties and make them thermally and chemically stable. Not all of these characteristics (for example, surface activity) are universal to all PFAS.

Table 6-2. Fluorine characteristics, resulting characteristics and properties of PFAS

Fluorine Characteristic	Description	Result	Resulting Property of PFAS
High electronegativity	Tendency to attract shared electrons in a bond	Strong C-F bond	Thermal stability
			Chemical stability (low reactivity)
		Polar bond with partial negative charge towards F	Strong acidity (low pKa)[1]
Low polarizability	Electron cloud density not easily impacted by the electric fields of other molecules	Weak intermolecular interactions (for example, van der Waals, hydrogen bonds)	Hydrophobic and lipophobic surfactant properties[2]
		Low surface energy	
Small size	Atomic radius of covalently bonded fluorine is 0.72 Å	Shields carbon	Chemical stability (low reactivity)

[1] When paired with an acid functional group such as a carboxylic or sulfonic acid

[2] When paired with a functional group that is hydrophilic (for example, a carboxylate)

Å = Angstrom

6.2.2 Acid Dissociation Constants

Knowing whether a chemical will dissociate in other liquids is important to understanding its fate and transport in the environment. The acid dissociation constant (K_a) is a quantitative measurement of the strength of an acid in solution, although it is usually presented in the form of the logarithmic constant (pK_a). The larger the value for pKa, the smaller the extent to which the chemical will dissociate at a given pH. Chemicals with small pKa values are called *strong acids* and those with large pKa values are called *weak acids*.

Many PFAAs, such as PFCAs and PFSAs, are strong acids due to the electron withdrawing effects of fluorine extending to their acid functional groups (Kissa 2001, Banks, Smart, and Tatlow 1994). As a result, most PFAAs readily dissociate in water and other environmental matrices. Therefore, at most environmentally relevant pHs, PFCAs and PFSAs are present in the dissociated anionic form rather than the acid form.

The acid and anionic forms have very different physical and chemical properties. For example, perfluorooctanoate anion is highly water soluble and has negligible vapor pressure, whereas perfluorooctanoic acid has very low water solubility and sufficient vapor pressure to partition out of water into air. It is essential to distinguish between the acid form and the anionic form when looking at physical and chemical properties or fate and transport evaluations.

Specific pKa values for PFAAs are generally not available. Limited model-predicted and experimental values are available for PFOA, and range from -0.5 to 3.8 (Burns et al. 2008; Kissa 2001; Barton, Kaiser, and Russell 2007; Goss 2008), suggesting that at nearly neutral pH (near pH = 7.0), PFOA will exist in the aqueous phase in anionic form and the amount of acid PFOA in most environmentally relevant systems will be negligible. A recent study estimates that the pKa values of PFBA, PFHxA, PFHpA, PFOA, PFNA, PFDA, and PFUnA are all less than 1.6 and pKa values of PFSAs are expected to be even lower (Vierke, Berger, and Cousins 2013).

6.2.3 Thermal and Chemical Stability

Terminal PFAAs, such as PFOA and PFOS, are extremely stable, thermally and chemically, and resist degradation and oxidation. Thermal stability of PFAAs is primarily attributable to the strength of the C-F bond in the fluoroalkyl tail (Kissa 2001). The stability is determined by the specific functional group that is attached to the fluoroalkyl tail. PFCAs and PFSAs are the most stable fluorinated surfactants. The acid forms of these PFAAs decompose at temperatures greater than 400°C, but complete mineralization occurs at temperatures greater than 1000°C. In a practical situation like a municipal incinerator, the mineralization temperature may be lower due to the presence of other substances that contain hydrogen. The thermal stability is lower for the salts of PFAA compounds and depends on which cation is the counter ion. For example, the 20% decomposition temperature of sodium perfluorooctanoate is 298°C, but is 341°C for lithium perfluorooctanoate (Kissa 2001). Additionally, salts of PFSAs are more thermally stable than the corresponding salts of PFCAs (Kissa 2001).

The strength of the C-F bond, shielding of carbon by fluorine, and inductive effects (caused by fluorine electronegativity) also lead to PFAS chemical stability. For example, electron-rich chemical species called nucleophiles normally would be attracted to the partial positive charge of carbon. If they can get close enough to the carbon to bond with it, this would eliminate a fluorine from the molecule, making it vulnerable to degradation. However, the size of the fluorine atoms surrounding the carbon prevents this from happening (Banks, Smart, and Tatlow 1994; Schwarzenbach, Gschwend, and Imboden 2003). This is why processes such as hydrolysis, which involve eliminating one or more fluorines, are ineffective at degrading PFAAs. Similarly, many PFAAs are resistant to degradation by oxidative processes that rely on a loss of electrons (Kissa 2001). PFAAs are also resistant to reductive processes, which involve gaining electrons. Despite having a high affinity for electrons, fluorine does not have vacant orbitals favorable for accepting additional electrons (Park et al. 2009).

6.2.4 Octanol/Water Partition Coefficient, K_{ow}

The octanol/water partition (K_{ow}) coefficient is sometimes used as a proxy for uptake in biological systems. The K_{ow} value is defined as “the ratio of a chemical’s concentration in the octanol phase to its concentration in the aqueous phase of a two-phase [octanol/water system]” (USEPA 2015d). The vapor pressure, melting point, and boiling point of neutral, volatile, nonpolymeric PFAS (for example, FTOH) can be measured, and K_{ow} can be either estimated or measured. The K_{ow} values that are typically tabulated for the PFCAs and PFSAs are for the acid form and are therefore not relevant because PFCAs and PFSAs are anionic at environmental pHs. Additionally, because many PFAS bind to proteins (proteinphiles), some PFAS may bioaccumulate by mechanisms other than those that drive more traditional hydrophobic contaminants (Ng and Hungerbühler 2013; 2014). Other PFAS may simply be detected in organisms due to ongoing exposures and their extended human half-lives (for example, concentrations in drinking water) (Wiesmueller 2012; Gyllenhammar et al. 2015). It should be noted that although the K_{ow} for some organic contaminants can be used for estimating K_{oc}, this cannot be performed for estimating values for PFAS.

7 Summary

This fact sheet addresses naming conventions and physical and chemical properties of some of the most commonly reported PFAS considering historical use, current state of science research related to environmental occurrence, and available commercial analyses. For naming conventions related to additional PFAS, refer to Buck et al. (2011). In general, values for physical and chemical properties of many nonpolymeric PFAS are not available. With the 2015 major global manufacturer phase-out of long-chain PFAAs and their potential precursors, such as those based on C8 chemistry (see *History and Use Fact Sheet*), replacement PFAS (for example, short-chain alternatives and nonpolymer perfluoropolyethers) have been commercially introduced (many following review by USEPA) and may continue to be developed. In the future, it may be necessary to expand the current naming conventions and acronym approaches to ensure that standardized naming is available for additional members of the PFAS class of compounds. Further, additional information on physical and chemical properties of these compounds may become available as increased numbers of PFAS are included in environmental and human health-related studies. Refer to the other PFAS fact sheets for further information on these properties and how they are practically applied.

8 References and Acronyms

The references cited in this fact sheet, and the other ITRC PFAS fact sheets, are included in one combined list that is available on the ITRC web site. The combined acronyms list is also available on the ITRC web site.

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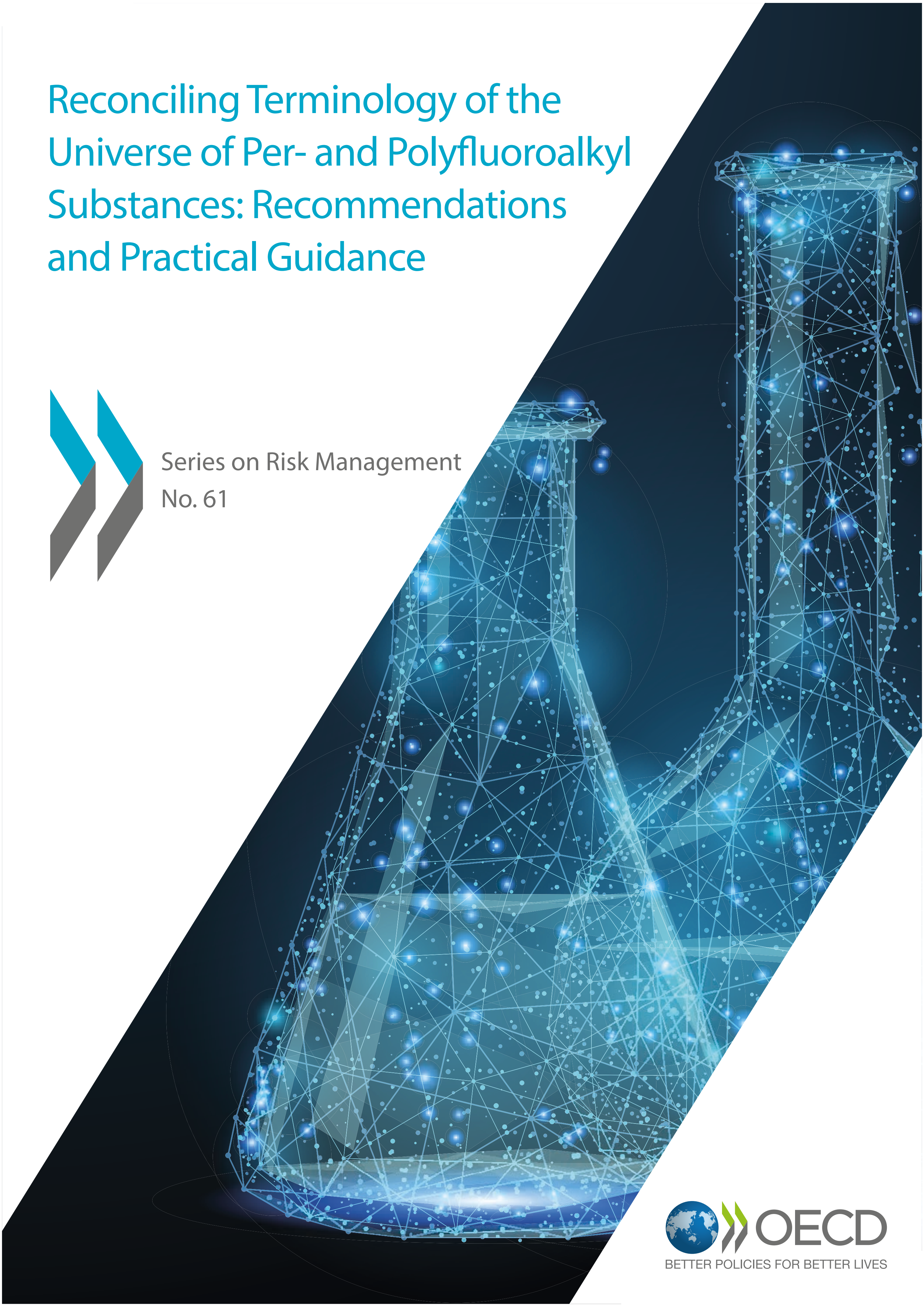
Reconciling Terminology of the Universe of Per- and Polyfluoroalkyl Substances: Recommendations and Practical Guidance

Series on Risk Management
No. 61



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Reconciling Terminology of the Universe of Per- and Polyfluoroalkyl Substances: Recommendations and Practical Guidance

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Executive Summary

This report summarizes recent efforts by the OECD/UNEP Global PFC Group between June 2018 and March 2021 in reviewing the universe and terminology of per- and polyfluoroalkyl substances (PFASs) to provide recommendations and practical guidance to all stakeholders with regard to the terminology of PFASs. In particular, this report highlights (1) a revised PFAS definition to comprehensively reflect the universe of PFASs and a comprehensive overview of the PFAS universe (Chapter 2), (2) practical guidance on how to use the PFAS terminology (Chapter 3), (3) a systematic approach to characterization of PFASs based on molecular structural traits to assist stakeholders, including non-experts, in making their own categorization based on their needs (Chapter 4), and (4) areas in relation to the PFAS terminology that warrant further development (Chapter 5). It should be noted that this report does not address the nomenclature and understanding of individual PFASs, including the sources of exposure and the actual composition of commercial products.

PFASs comprise a class of synthetic compounds that have attracted much public attention since the late 1990s and early 2000s, when the hazards and ubiquitous occurrence of two PFASs, perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS), started to be reported and recognized. Since then, research and risk management measures have expanded from these two PFASs to a wider range of PFASs. Early communications used many different terminologies (e.g. per- and polyfluorinated chemicals, perfluorinated organics, perfluorochemical surfactants, highly fluorinated compounds). In 2011, to unify and harmonize communication on PFASs, Buck et al. published a milestone paper, providing a first clear structural definition of PFASs and recommendations on names and acronyms for over 200 individual PFASs.

Currently, there is a growing interest by regulators and scientists across the globe to assess legacy and novel PFASs. In 2018, the OECD/UNEP Global PFC Group prepared a new list of PFASs that may have been on the global market. In total, a set of substances with over 4730 CAS numbers have been identified, including substances that contain such fully fluorinated carbon moieties, but do not meet the PFAS definition in Buck et al. (2011) due to a lack of a –CF3 group in the molecular structures. In addition, recent advancement of non-target screening analytical techniques using high-resolution mass spectrometry has enabled identification of many unknown substances in different environmental and product samples. The identification of these substances motivates the present work to reconcile the terminology of the universe of PFASs, including a renewed look at the PFAS definition in Buck et al. (2011).

It is key to have a coherent and consistent logic behind the PFAS definition to adequately reflect all compounds with the same structural traits, i.e. the PFAS universe. Building on the OECD 2018 PFAS List and recent non-target screening studies, Chapter 2 first identifies four major gaps in the previous PFAS definition by Buck et al. (2011) in representing the PFAS universe. Then, Chapter 2 recommends a revised PFAS definition, with detailed elaboration on individual changes provided:

PFASs are defined as fluorinated substances that contain at least one **fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it)**, i.e. with a few noted exceptions, any chemical with at least a perfluorinated methyl group ($–CF_3$) or a perfluorinated methylene group ($–CF_2–$) is a PFAS.

The rationale behind the revision is to have a general PFAS definition that is coherent and consistent across compounds from the chemical structure point of view and is easily implementable for distinguishing between PFASs and non-PFASs, also by non-experts. The decision to broaden the definition compared to Buck et al. is not connected to decisions on how PFASs should be grouped in regulatory and voluntary actions. Based on the revised definition of PFASs, Chapter 2 further illustrates (1) how PFASs fit into organofluorine compounds, (2) a comprehensive overview of PFAS groups, their structural traits, examples and notes on whether common nomenclatures (including acronyms) exist for them, and (3) some common synthesis routes of different individual or groups of PFASs.

As PFASs are a chemical class with diverse molecular structures and physical, chemical and biological properties, it is highly recommended that such diversity be properly recognized and communicated in a clear, specific and descriptive manner. The term “PFASs” is a broad, general, non-specific term, which does not inform whether a compound is harmful or not, but only communicates that the compounds under this term share the same trait for having a fully fluorinated methyl or methylene carbon moiety. In particular, Chapter 3 provides practical guidance to governments and other stakeholders on how to use the PFAS terminology, starting from the distinction between the general definition and user-specific working scopes of PFASs. In particular, the general definition of PFASs is based on molecular structure alone and serves as a starting and reference point to guide individual users to have a comprehensive understanding of the PFAS universe and to keep the big picture of the PFAS universe in mind. At the same time, individual users may define their own working scope of PFASs for specific activities according to their specific needs by combining the general definition of PFASs with additional considerations (e.g. specific properties, use areas). This report does not make any recommendation on how working scopes should be set up, in terms of which factors to be considered (which depends highly on specific local context), nor on PFAS grouping. However, when a working scope of PFASs is used, this report highly recommends that users clearly provide the context and rationale for selecting their PFAS working scope in order to provide transparency and avoid confusion by others. Further, the report recommends to use and build upon existing common terminologies such as in this report, in Buck et al. (2011) and common practices in organic chemistry as set by IUPAC and CAS, unless it is essential to deviate from existing naming conventions, in order to keep the consistence and coherence of the PFAS terminology.

As users often define their own working scope of PFASs according to their specific needs, they need to characterize PFASs based on pre-defined traits and categorize them (e.g. whether a compound with certain traits falls or does not fall into their working scope). However, given the high complexity and diversity of PFASs, it can be a challenging task to characterize and categorize PFASs based on chemical structures in a coherent and consistent manner, particularly for non-experts. In addition, different users may have very different needs, and there is no single categorization/grouping system that can meet all needs. Therefore, Chapter 4 provides a standardized approach for systematic characterization of different PFASs based on molecular structural traits that will allow stakeholders to make their own categorization in a coherent and consistent manner. In addition to the manual application of the system to characterize and categorize PFASs, the elements presented here may also be used as inputs for developing cheminformatic tools that would allow automated characterization and categorization of PFASs.

While this report makes advancement on several important points regarding PFAS terminology and practical guidance of how to use the PFAS terminology, Chapter 5 also recognizes four areas that warrant further work, in order to facilitate clear and unambiguous communication of PFASs and beyond: (1) a centralized PFAS nomenclature database/platform; (2) further development of cheminformatics-based tools for automated systematic characterizing and categorizing PFASs; (3) further work on the characterization and reporting of polymers; and (4) work on organofluorine compounds other than PFASs including many fluorinated aromatics.

List of Acronyms

ADONA	Ammonium 4,8-dioxa-3H-perfluorononanoate
Br	Bromine atom
CAS	Chemical Abstracts Service
CAS Nos.	Chemical Abstracts Service registry numbers
Cl	Chlorine atom
CTFE	Chlorotrifluoroethylene
ECHA	European Chemicals Agency
ETFE	Ethylene-tetrafluoroethylene copolymer
EU	European Union
FASAs	Perfluoroalkane sulfonamides
FASEs	Perfluoroalkane sulfonamidoethanols
FEP	Fluorinated ethylene propylene co-polymer
FPs	Fluoropolymers
FTABs	Fluorotelomer sulfonamide alkylbetaines
FTEOs	Fluorotelomer ethoxylates
FTIs	Fluorotelomer iodides
FT(MA)ACs	Fluorotelomer (meth)acrylates
FTOs	Fluorotelomer olefins
FTOHs	Fluorotelomer alcohols
FTSAs	Fluorotelomer sulfonic acids
HFCs	Hydrofluorocarbons
HFEs	Hydrofluoroethers
HFOs	Hydrofluoroolefins
HFP	Hexafluoropropylene
HFPO	Hexafluoropropylene oxide
HFPO-DA	Hexafluoropropylene oxide dimer acid
H	Hydrogen atom
I	Iodine atom
ICCM	International Conference on Chemicals Management
InChI	International chemical identifier

InChIKey	A hashed version of the full InChI
ITRC	Interstate Technology & Regulatory Council in the United States
IUPAC	International Union of Pure and Applied Chemistry
OBS	Sodium *p*-perfluorous noenoxybenzenesulfonate
OECD	Organisation for Economic Co-operation and Development
PACFs	Perfluoroalkanoyl fluorides
PASFs	Perfluoroalkane sulfonyl fluorides
PCTFE	Polychlorotrifluoroethylene
PFA	Perfluoroalkoxyl polymer
PFAAs	Perfluoroalkyl acids
PFAIs	Perfluoroalkyl iodides
PFASs	Per- and polyfluoroalkyl substances
PFCAs	Perfluoroalkyl carboxylic acids
PFdiCAs	Perfluoroalkyl dicarboxylic acids
PFdiSAs	Perfluoroalkane disulfonic acids
PFECAs	Perfluoroalkylether carboxylic acids
PFEI	Perfluoroethyl iodide
PFESAs	Perfluoroalkylether sulfonic acids
PFHxS	Perfluorohexane sulfonic acid
PFOA	Perfluorooctanoic acid
PFOS	Perfluorooctane sulfonic acid
PFPAs	Perfluoroalkyl phosphonic acids
PFPEs	Perfluoropolyethers
PFPIAs	Perfluoroalkyl phosphinic acids
PFSAs	Perfluoroalkane sulfonic acids
PFSIAs	Perfluoroalkane sulfinic acids
PolyFCAs	Polyfluoroalkyl carboxylic acids
PolyECAs	Polyfluoroalkylether carboxylic acids
PolyESAs	Polyfluoroalkylether sulfonic acids
POPs	Persistent Organic Pollutants
POSF	Perfluoroctane sulfonyl fluoride
PPVE	Perfluoropropylvinyl ether
PTFE	Polytetrafluoroethylene
PVDF	Polyvinylidene fluoride
PVF	Polyvinyl fluoride
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals (EC 1907/2006)
SaMPAPs	Perfluorooctane sulfonamidoethanol phosphate esters
SFAs	Semifluorinated alkanes

SMILES	Simplified molecular input line entry specification
TFE	Tetrafluoroethylene
THV	Terpolymer of tetrafluoroethylene, hexafluoropropylene and vinylidene fluoride
UNEP	United Nations Environment Programme
VDF	Vinylidene fluoride

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FIGURES

TABLES

Chapter 1. Background, motivation and scope

The OECD/UNEP Global PFC[1] Group was established to respond to the Resolution II/5 adopted at the second session of the UN International Conference on Chemicals Management (ICCM 2) in 2009, which calls upon intergovernmental organizations, governments and other stakeholders to "consider the development, facilitation and promotion in an open, transparent and inclusive manner of national and international stewardship programmes and regulatory approaches to reduce emissions and the content of relevant perfluorinated chemicals of concern in products and to work toward global elimination, where appropriate and technically feasible". Further work on this resolution was reaffirmed in Resolution III/3 adopted at ICCM 3 in 2012 noting that a significant need remains for additional work to support implementation of Resolution II/5. This report is prepared within the framework of the Group. For more details on the Group and its work, see the OECD PFAS web portal (https://oe.cd/2M9).

This report summarizes recent efforts by the OECD/UNEP Global PFC Group between June 2018 and March 2021 in reviewing the universe and terminology of per- and polyfluoroalkyl substances (PFASs[2]) to provide recommendations and practical guidance to all stakeholders (governments, industry, academia, civil society organizations, etc.) regarding the terminology of PFASs. In particular, this report highlights (1) a revised PFAS definition to comprehensively reflect the universe of PFASs and a comprehensive overview of the PFAS universe (Chapter 2), (2) a practical guidance on how to use the PFAS terminology, from a general PFAS definition to user-specific working scopes to naming conventions of individual PFASs (Chapter 3), (3) a systematic approach to characterization of PFASs based on molecular structural traits to assist stakeholders, including non-experts, in making their own categorization based on their needs (Chapter 4), and (4) areas in relation to the PFAS terminology that warrant future work (Chapter 5). It should be noted that this report does not address the nomenclature and understanding of individual PFASs, including the sources of exposure and the actual composition of commercial products. It also does not address organofluorine compounds other than PFASs.

PFASs comprise a class of synthetic compounds that have attracted much public attention since the late 1990s and early 2000s, when the hazards and ubiquitous occurrence of two PFASs, perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS), started to be reported and recognized. Since then, research and risk management measures have expanded from these two PFASs to a wider range of PFASs [e.g. 3M's voluntary global phase-out of C_{6-10} perfluoroalkane sulfonic acids (PFSAs), PFOA and related chemistries in 2000–2002]. It is noted that early communications used many different terminologies (e.g. per- and polyfluorinated chemicals, perfluorinated organics, perfluorochemical surfactants, highly fluorinated compounds).

In 2011, to unify and harmonize communication on PFASs, Buck et al. published a milestone paper on a first comprehensive overview of PFASs detected in the environment, wildlife, and humans. It provided a first clear structural definition of PFASs. A particular emphasis of Buck et al. (2011) was placed on long-chain perfluoroalkyl acids [PFAAs, i.e., perfluoroalkyl carboxylic acids (PFCAs) with seven or more perfluorinated carbons and PFSAs with six or more perfluorinated carbons][3], substances related to the long-chain PFAAs, and substances intended as alternatives to the long-chain PFAAs or their precursors[4].

In addition, Buck et al. (2011) provided a list of 42 families and subfamilies[5] of PFASs and 268 selected individual compounds, including recommended names and acronyms, structural formulas, and Chemical Abstracts Service registry numbers (CAS Nos.).

Today, several long-chain PFAAs have been recognized as global contaminants of high concern. For example, PFOS, its salts, and perfluorooctane sulfonyl fluoride (POSF[6]), as well as PFOA, its salts, and PFOA-related compounds have been listed under the Stockholm Convention on Persistent Organic Pollutants (POPs) for global actions. In addition, the POPs Review Committee to the Stockholm Convention decided in 2019 to recommend that the Conference of the Parties to the Stockholm Convention consider listing perfluorohexane sulfonic acid (PFHxS, C_6 PFSA), its salts and PFHxS-related compounds at its tenth meeting. In response to these actions, an industrial transition has taken place to replace long-chain PFAAs and their precursors with alternative chemicals, many of which are still PFASs, including short-chain PFAAs and their precursors as well as perfluoroalkylether-based substances (for examples, see Buck et al., 2011, Wang et al., 2013, 2016 and references therein). It is noted that there is a growing interest by regulators[7] and scientists across the globe to assess legacy and novel PFASs other than long-chain PFAAs and their well-known precursors.

In particular, various efforts have been made to identify overlooked PFASs. In 2018, the OECD/UNEP Global PFC Group prepared a new list of PFASs[8] that may have been on the global market using a systematic search of substances that have a $–C_nF_{2n}–$ (n ≥3) or $–C_nF_{2n}OC_mF_{2m}–$ (n and m ≥1) moiety in different publicly accessible sources. In total, a set of substances with over 4730 CAS Nos. have been identified, including substances that contain fully fluorinated carbon moieties and are structurally similar to or related to commonly known PFASs [e.g. perfluoroalkyl dicarboxylic acids (PFdiCAs) to PFCAs], but do not meet the PFAS definition in Buck et al. (2011) due to a lack of a $–CF_3$ group in the molecular structures (for more details, see Section 2.2). Meanwhile, recent advancement of non-target screening analytical techniques using high-resolution mass spectrometry has enabled identification of many unknown substances in different environmental and product samples [e.g. $H–(CF_2CH_2)_n–CF_2COOH$ by Newton et al. (2017)].

The identification of overlooked PFASs motivates the present work to reconcile the terminology of the universe of PFASs, including a renewed look at the PFAS definition in Buck et al. (2011) (see Chapter 2). In light of these newly identified substances and building on existing common terminology provided in Buck et al. (2011), this report and others, this report also looks into practical guidance on how to use the PFAS terminology, including uses of user-specific working scopes (see Chapter 3). In addition, the OECD 2018 PFAS List and recent non-target screening studies show the complexity and diversity of the PFAS universe, resulting in challenges for non-experts in conducting their own categorization of PFASs based on molecular structures. Therefore, this report also looks into systematic approaches to characterization and categorization of PFASs to assist stakeholders in making their own categorization based on their needs (see Chapter 4). Further, this report highlights open questions in relation to PFAS terminology for future consideration (see Chapter 5).

Notes

[1] "PFCs" here refer to "per- and polyfluorinated chemicals", and not to "perfluorocarbons". As stated below, "per- and polyfluorinated chemicals" was a term commonly used before the term "per- and polyfluoroalkyl substances" was recommended by Buck et al.. As it is part of the Group official name, it remains unchanged.

[2] This report uses the acronym “PFASs” for “per- and polyfluoroalkyl substances” as stated in Buck et al. (2011), and its corresponding singular form “PFAS” refers to either a perfluoroalkyl or polyfluoroalkyl substance. It is noted that there is a notion of using “PFAS” as the acronym for both the singular and plural forms. This report does not make any recommendation to address this notion, as it is a trivial point that is difficult for everyone to comprehend, particularly for non-PFAS experts and non-English native speakers. While recognizing that readers may make their own decision which acronym they would use, this report encourages readers to always use the acronym consistently in their documents (for more details on practice guidance on how to identify and use the PFAS terminology, see Section 3.2 below).

[3] Note that the definition of “long-chain PFAAs” here is based on the OECD definition (https://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/aboutpfass/), and the definitions of “long-chain PFAAs” may differ by jurisdiction.

[4] PFAA precursors refer to chemicals that can transform and form PFAAs in the environment and biota.

[5] Note that in the literature, some authors have used other taxonomy terminologies, e.g. “groups and subgroups” instead of “families and subfamilies”. This report does not propose a new taxonomy terminology for PFASs, but makes some practical guidance on how to use taxonomy terminologies (see Chapter 3 below).

[6] Note that the acronym “POSF” here is used in accordance with the recommendations by Buck et al. (2011), whereas under the Stockholm Convention, another acronym “PFOSF” is used.

[7] For example, five European Union (EU) member states have agreed to prepare a joint REACH restriction proposal to limit the risks to the environment and human health from the manufacture and use of a wide range of PFASs, and thus launched a public call for evidence in May 2020 with regard to substances that contain at least one aliphatic $–CF_2–$ or $–CF_3$ element. For more details, see https://echa.europa.eu/hot-topics/perfluoroalkyl-chemicals-pfas. In addition, multiple PFASs other than long-chain PFAAs and their precursors are listed in ECHA’s Public Activities Coordination Tool (PACT) to be assessed by ECHA or EU member states (https://echa.europa.eu/pact).

[8] The Excel Spreadsheet version of the OECD 2018 PFAS list can be found at https://www.oecd.org/chemicalsafety/risk-management/global-database-of-per-and-polyfluoroalkyl-substances.xlsx. In addition, several other entities have curated the OECD 2018 PFAS list into their databases, with features such as an easier overview of chemical structures and links to other information, including the US EPA CompTox Chemicals Dashboard (https://comptox.epa.gov/dashboard/chemical_lists/PFASOECD), NORMAN Network (https://www.norman-network.com/?q=suspect-list-exchange) and PubChem (https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101).

In addition, the US EPA CompTox Chemicals Dashboard also provides a number of other PFAS lists intended to address different research and regulatory interests, including PFASSTRUCT that is compiled from all the records with a structure assigned in the Dashboard using a pre-defined set of substructural filters and contains over 8000 compounds, as of 23 November, 2020 (for more details including the list of substructural filters, see https://comptox.epa.gov/dashboard/chemical_lists/PFASSTRUCT). Note that these lists may also include substances that are not regarded as PFASs in accordance with the revised PFAS definition below.

Chapter 2. Reconciling Terminology of the Universe of PFASs

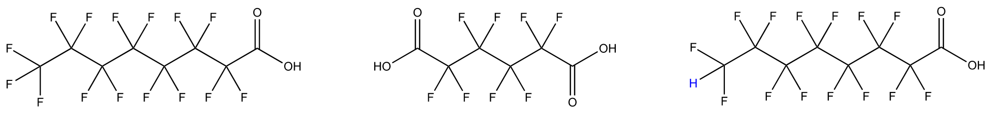
2.1. The previous PFAS definition in Buck et al. (2011)

In Buck et al. (2011), **PFASs** were defined as "the **highly fluorinated aliphatic substances** that contain **1 or more C atoms** on which all the H substituents (present in the nonfluorinated analogues from which they are notionally derived) have been replaced by F atoms, in such a manner that they contain the perfluoroalkyl moiety **C_nF_{2n+1}–**" (i.e. must contain at least $-CF_3$). The definition highlights the presence of at least one fully fluorinated saturated carbon atom in the PFAS molecules.

2.2. Gaps in the previous PFAS definition by Buck et al. (2011)

It is key to have a coherent and consistent logic behind the PFAS definition to reflect all compounds with shared structural traits, i.e. the PFAS universe. Building on the OECD 2018 PFAS List and recent non-target screening studies, this section identifies gaps in the previous PFAS definition by Buck et al. (2011) in representing the PFAS universe. Note that the gaps identified in this report are not exhaustive and additional gaps in the PFAS definition may be identified in the future; therefore, an iterative approach is guaranteed to ensure the consistency between the PFAS universe and terminology when new knowledge of gaps in the PFAS definition is generated.

Case 1: The fully fluorinated saturated carbon moiety[9] is connected with functional groups on both ends, including having a single H/Br/Cl atom on one end. As such, it does not meet the structural requirement of **"$–C_nF_{2n+1}$"** in the previous definition. In the example of a1 in Figure 1, it is a PFdiCA with a similar structure to PFCAs (e.g. PFOA in the example of A in Figure 1), but having carboxylic groups on both ends of the perfluoroalkanediyl moiety. In addition, for the example of a2 in Figure 1, it would meet the previous definition if the H atom was moved to a secondary carbon atom (i.e. $CF_3CFHCF_2CF_2CF_2CF_2CF_2COOH$, a positional isomer).



A. PFOA, CAS No. 335-67-1　a1. CAS No. 336-08-3　a2. CAS No. 13973-14-3

Figure 1. PFOA and examples of substances with similar molecular structures, but having functional groups (including single atoms such as hydrogen) on both ends of the perfluoroalkanediyl moiety.

Furthermore, functionalized fluoropolymers and perfluoropolyethers[10] (i.e. those that have functional groups on both ends of the polymer backbone, e.g. Fomblin HC/P2 1000[11]) do not meet the structural requirement of **"$–C_nF_{2n+1}$"** in the previous definition, whereas their closely related analogues with only fluorine atoms on each end of the polymer backbone would meet the previous definition.

Case 2: The substance is a fully fluorinated aliphatic cyclic compound which may or may not have a fully fluorinated alkyl side chain. As such, it may not meet the structural requirement of **"$–C_nF_{2n+1}$"** in the previous definition. For example, b1 in Figure 2 meets the previous definition, whereas its shorter-chain homologue, b2 in Figure 2, does not meet the previous definition.

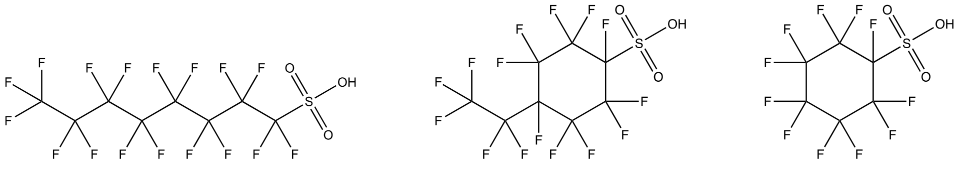

B. PFOS, CAS No. 1763-23-1 **b1. CAS No. 646-83-3** **b2. CAS No. 2106-55-0**

Figure 2. PFOS, an example of a cyclic PFSA, and a shorter-chain homologue of the cyclic PFSA

Case 3: The functional group contains an aromatic ring. Thus, it may not meet the term **"aliphatic substances"** in the previous definition, although the example of c1 in Figure 3 is a derivative of 6:2 fluorotelomer iodide, i.e. a 6:2 fluorotelomer-based compound.

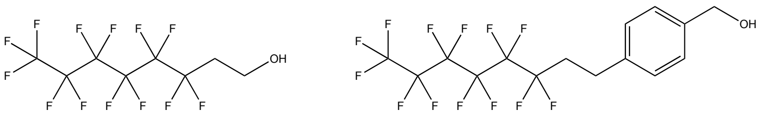
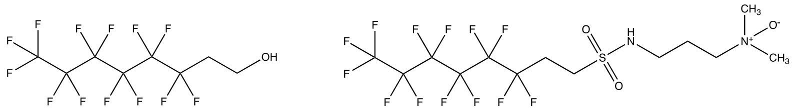

C. 6:2 FTOH, CAS No. 647-42-7 **c1. CAS No. 356055-76-0**

Figure 3. 6:2 FTOH, and a 6:2 fluorotelomer iodide derivative with one aromatic ring in the functional group

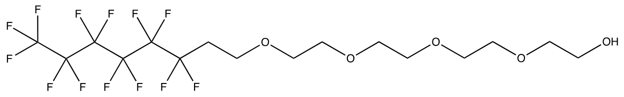
Case 4: The description "highly fluorinated" in the previous definition is an ambiguous, problematic term. It cannot and should not be literally translated to, e.g., the weight percentage of fluorine atoms in the molecules, using three 6:2 fluorotelomer-based compounds as an example (see Figure 4):

- $C_6F_{13}C_2H_4OH$ (6:2 FTOH; CAS No. 647-42-7) has a fluorine content of 67.8 wt%,
- $C_6F_{13}C_2H_4SO_2NHC_3H_6N(O)(CH_3)_2$ used in Forafac® 1183 (CAS No. 80475-32-7) has a fluorine content of 46.7 wt%, and
- 6:2 fluorotelomer ethoxylates [$C_6F_{13}–(CH_2CH_2O)_n–H$, n = 0–13] in a commercial product (Frömel and Knepper, 2010) would have even lower fluorine content when n>4.

But they are all 6:2 fluorotelomer-based compounds and may act as precursors to perfluorohexanoic acid (PFHxA) in the environment and biota.



6:2 FTOH, CAS No. 647-42-7, F(mass%) = 67.8%   **CAS No. 80475-32-7, F(mass%) = 46.7%**



CAS No. 1663471-34-8, F(mass%) = 45.7%

Figure 4. 6:2 FTOH and two 6:2 fluorotelomer derivatives, and their corresponding fluorine contents

2.3. A revised PFAS definition

Therefore, there is a need to revisit the previous definition in Buck et al. (2011) to address these gaps (i.e. the previous definition was not comprehensive enough and contained ambiguous descriptions). A clear distinction of the logical relationship needs to be made here: the intention of the revision of the PFAS definition is not to expand the PFAS universe, but to comprehensively reflect it. More concretely, the rationale behind the revision is to have a general PFAS definition that is coherent and consistent across compounds from the chemical structure point of view and is easily implementable for distinguishing between PFASs and non-PFASs, also by non-experts.

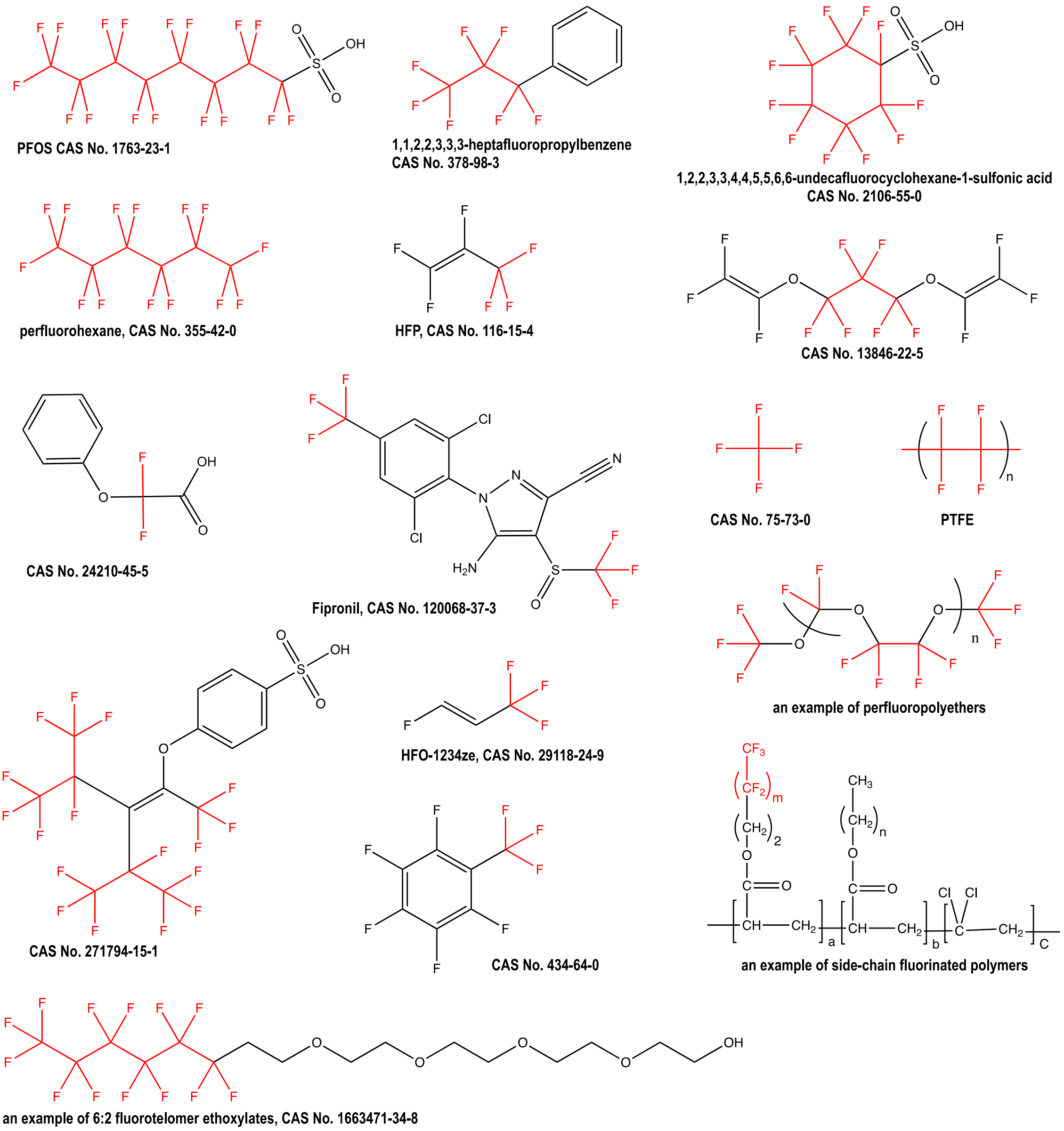
This revised PFAS definition reads,

PFASs are defined as fluorinated substances that contain at least one **fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it)**, i.e. with a few noted exceptions, any chemical with at least a perfluorinated methyl group (–CF_3) or a perfluorinated methylene group (–CF_2–) is a PFAS**.**

Both a perfluorinated methyl group and a perfluorinated methylene group are saturated and aliphatic. Note that the carbon in a R–CF_2–O– or R–CF_2–Si– group (R ≠ H/Cl/Br/I) is a perfluorinated methylene carbon. A perfluorinated methylene group may also be represented as “>CF_2”, where “>” denotes two single bonds. A fully fluorinated carbon that is bound to the rest of the molecule by a double bond is a perfluorinated methyl*idene* carbon atom (=CF_2). This distinction is important. Further, a perfluorinated methine carbon moiety (>CF–) alone does not meet this revised PFAS definition.

It should be noted that this general PFAS definition is based only on chemical structure, and the decision to broaden this definition compared to Buck et al. (2011) is not connected to decisions on how PFASs should be grouped and managed in regulatory and voluntary actions. For further practical guidance on how to use this general PFAS definition, see Section 3.1.

Figure 5 illustrates substances that are PFASs, and Figure 6 shows those that are not PFASs. Note that tetrafluoroethylene (TFE, CAS No. 116-14-3, CF_2=CF_2) is not a PFAS as both fully fluorinated carbon atoms are unsaturated; its longer-chain homologue hexafluoropropylene (HFP, CAS No. 116-15-4, CF_2=CF–CF_3) is a PFAS due to the presence of a fully fluorinated methyl carbon atom (–CF_3).



PFOS CAS No. 1763-23-1

1,1,2,2,3,3,3-heptafluoropropylbenzene
CAS No. 378-98-3

1,2,2,3,3,4,4,5,5,6,6-undecafluorocyclohexane-1-sulfonic acid
CAS No. 2106-55-0

perfluorohexane, CAS No. 355-42-0

HFP, CAS No. 116-15-4

CAS No. 13846-22-5

CAS No. 24210-45-5

Fipronil, CAS No. 120068-37-3

CAS No. 75-73-0

PTFE

an example of perfluoropolyethers

CAS No. 271794-15-1

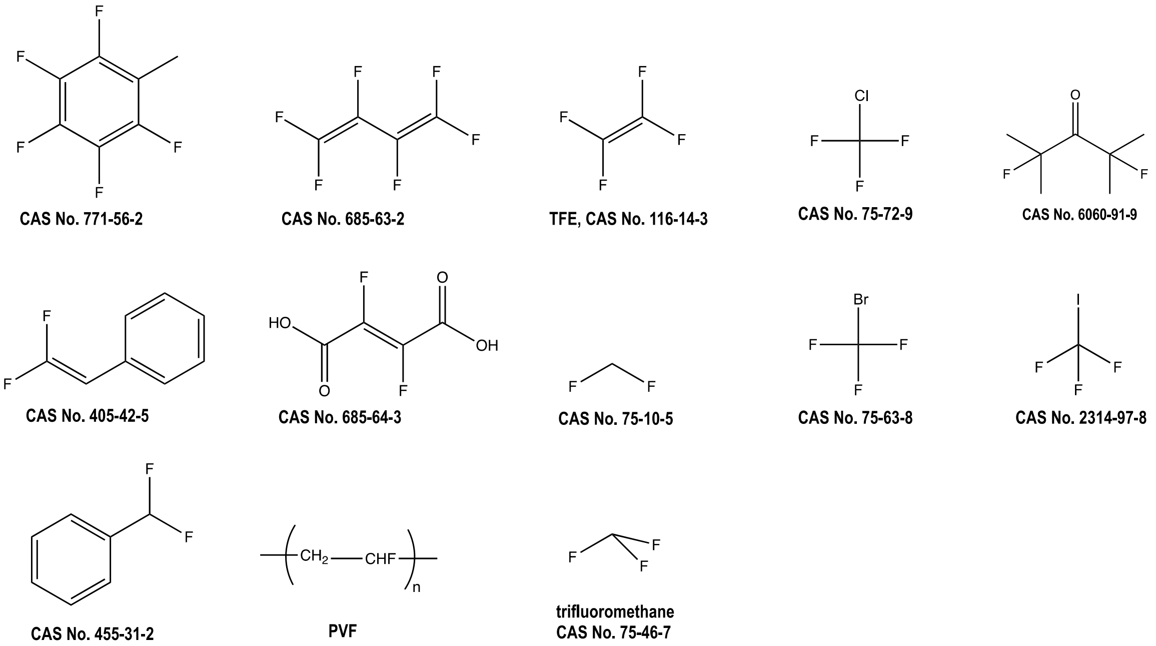
HFO-1234ze, CAS No. 29118-24-9

CAS No. 434-64-0

an example of side-chain fluorinated polymers

an example of 6:2 fluorotelomer ethoxylates, CAS No. 1663471-34-8

Figure 5. Examples of PFASs. The fully fluorinated methyl or methylene carbon atoms are highlighted in red.



CAS No. 771-56-2

CAS No. 685-63-2

TFE, CAS No. 116-14-3

CAS No. 75-72-9

CAS No. 6060-91-9

CAS No. 405-42-5

CAS No. 685-64-3

CAS No. 75-10-5

CAS No. 75-63-8

CAS No. 2314-97-8

CAS No. 455-31-2

PVF

trifluoromethane
CAS No. 75-46-7

Figure 6. Examples of compounds that are not PFASs due to a lack of fully fluorinated methyl or methylene carbon atoms.

The rationale for making such changes is detailed as follows.

- **Change from "highly fluorinated aliphatic substances" to "fluorinated substances that contain at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it)":**

  First, the qualifier "highly" is removed from the definition, as it is not meaningful when the fluorinated carbon chain can cleave from the substance to produce a new molecule that is more highly fluorinated [see Section II in FOEN (2017) and references therein].

  Second, the term "aliphatic" is removed from the definition. As shown in Case 3 in Figure 3, aromatic ring(s) may be present as a part of the functional group connecting to a fully fluorinated methyl or methylene carbon moiety. Using the previous definition by Buck et al. (2011), such compounds would not be recognized as PFASs, whereas compounds with similar structures but without aromatic ring(s) are recognized as PFASs. This may easily create confusion as to when a substance is or is not a PFAS, particularly for non-experts. The change of wording here is also to make the definition more straightforward. At the same time, the new wording "substances that contain at least one fully fluorinated methyl or methylene carbon atom" means that this revised definition is still constrained to the key trait of having an aliphatic fully fluorinated saturated carbon moiety and excluding those fluorinated aromatics that only have fluorine directly attached to the aromatic rings. Overall, this revised definition includes side-chain fluorinated aromatics [i.e. aromatics that have one or more aliphatic fully fluorinated saturated carbon moiety on the side chain(s) attached to the aromatic ring(s), an analogy to "side-chain fluorinated polymers"[12] as in Buck et al. 2011] as PFASs; for examples, see c1 in Figure 3 and Figure 7 below.

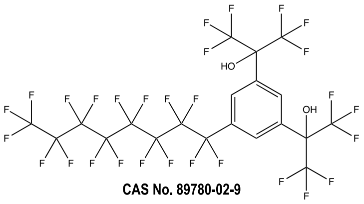


Figure 7. An example of side-chain fluorinated aromatics.

- **Change from "the perfluoroalkyl moiety C_nF_{2n+1}–" to "at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it)":**

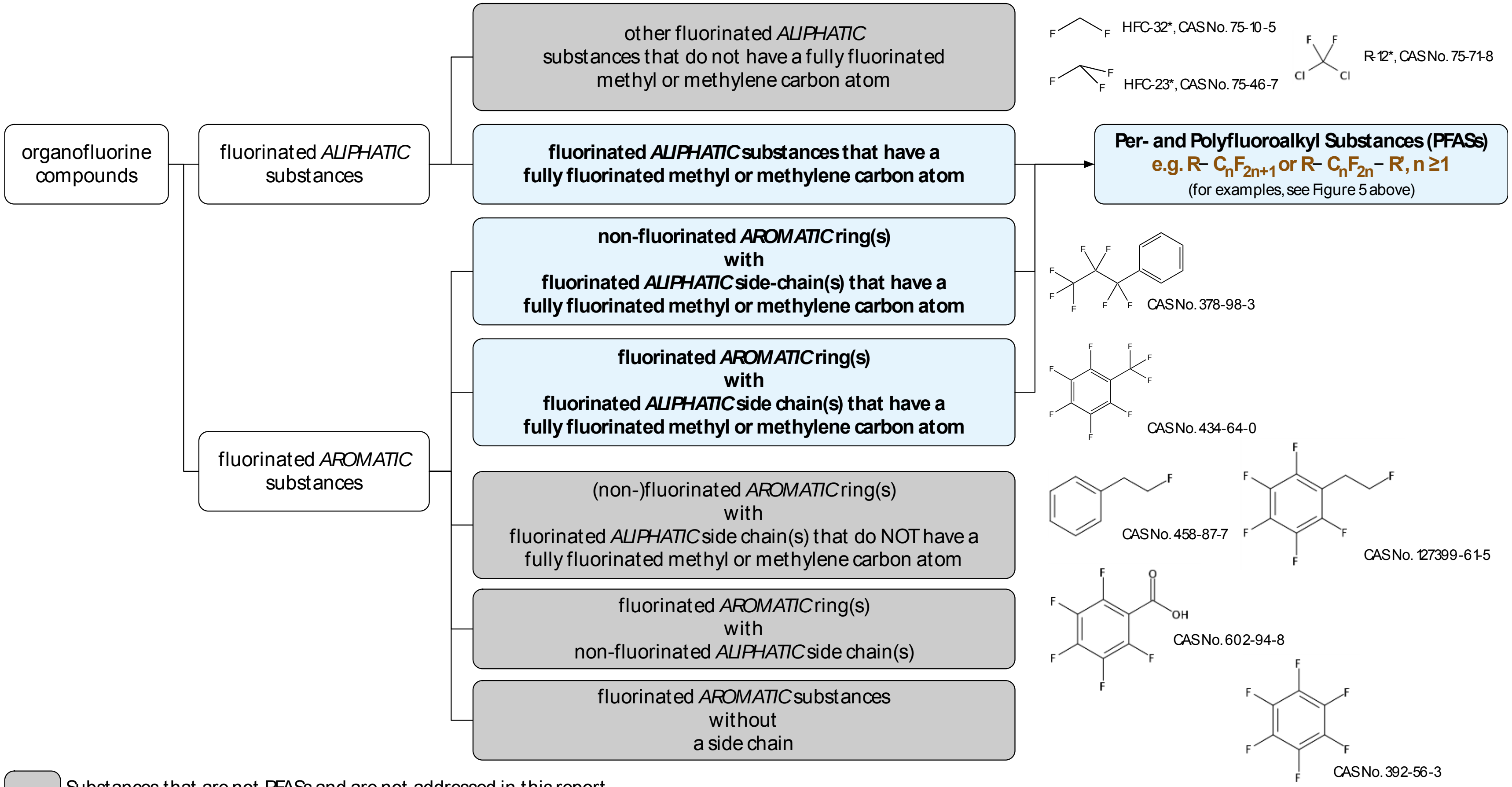
  This change is to accommodate those that have functional groups on both ends of the fully fluorinated saturated carbon moieties (Case 1) and those that have cyclic structure(s) at the end of the fully fluorinated saturated carbon moieties (Case 2).

  In addition, two more specific descriptions are made here to make the definition clearer. First, the term "methyl or methylene carbon atom" is added to describe the fully fluorinated saturated carbon moiety, which was not clear from the description "that contain only 1 or more C atoms on which all the H substituents … have been replaced by F atoms", but only implicitly mentioned in the description "in such a manner that they contain the perfluoroalkyl moiety C_nF_{2n+1}–". Second, adding "without any H/Cl/Br/I atom attached to it" highlights that the carbon atom is considered non-fully fluorinated, when a H/Cl/Br/I atom is attached to it.

2.4. A comprehensive overview of the PFAS universe

Based on this revised definition of PFASs, a first scheme can be drawn to illustrate how PFASs fit into organofluorine compounds (see Figure 8). It can be seen that besides PFASs, there are many other organofluorine compounds, including (1) fluorinated aliphatic substances that do not have a fully fluorinated methyl or methylene carbon atom [e.g. trifluoromethane (HFC-23) and difluoromethane (HFC-32)], (2) fluorinated aromatic substances with no side chain(s) (e.g. hexafluorobenzene, CAS No. 392-56-3), and (3) fluorinated aromatic substances with non-fluorinated side chain(s) (e.g. pentafluorobenzoic acid, CAS No. 602-94-8). These other organofluorine compounds are beyond the scope of this report, and future work on them is encouraged.

Looking at the PFAS universe, it is a highly complex chemical class with compounds having diverse functional groups attached to the fully fluorinated saturated carbon moiety/-ies. Figure 9 provides a comprehensive overview of PFAS groups, their structural traits, examples and notes on whether common nomenclatures (including acronyms) exist for them, building on Buck et al. (2011) and the OECD 2018 List. Figure 10 illustrates some common synthesis routes of different individual or groups of PFASs based on publicly accessible sources. It should be noted that, while Figures 9 and 10 aim to be comprehensive, they are by no means exhaustive. For more information on individual PFAS groups (e.g. major compounds in the group, synthesis routes, major uses, regulatory status, environmental occurrence, etc.), readers may consult the PFAS Fact Cards published on the OECD PFAS Web portal: https://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/.



▨ Substances that are not PFASs and are not addressed in this report

* HFC-32, HFC-23 and R-12 are not PFASs, despite the presence of moieties such as $-CF_2-$ or $-CF_3$, because not all H on the fluorinated carbon atom are replaced by F, i.e., they do not have a fully fluorinated carbon atom.

Figure 8. An illustrative scheme of how PFASs fit into the universe of organofluorine compounds

Note: This figure is intended to be comprehensive, but not exhaustive; in other words, there are other groups of PFASs that are not captured in this figure.

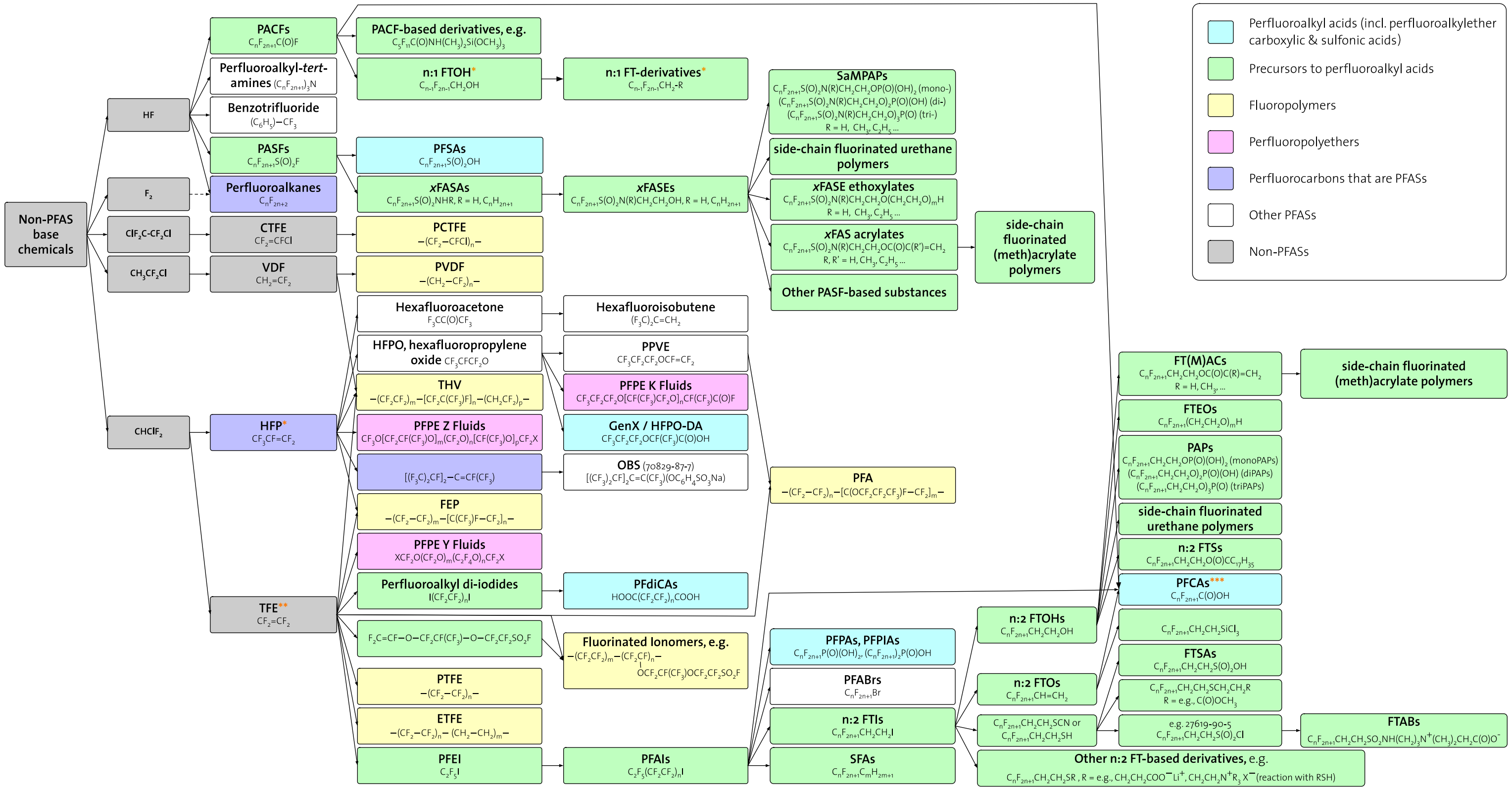
* It is recommended that *poly*fluoroalkyl acids use the acronym *Poly*FAA to better distinguish from *per*fluoroalkyl acids. Depending on the fluorination degree and location, *poly*fluoroalkyl carboxylic acids may either be highly persistent themselves, or act as precursors to other PFAAs such as PFdiCAs, under natural conditions.

** Strictly speaking, these substances are not fluorotelomers, as they are not derived from the telomerization process. Despite this, they are termed here "n:1 fluorotelomer-based" substances for readability. Future work may consider to identify more proper terminology for this group of PFASs.

*** Depending on the type of linkages between fluorinated side chain(s) and aromatic ring(s), some side-chain fluorinated aromatics may act as precursors to PFAAs or PFEAAs.

**** Depending on the molecule structure, one may belong to PFAAs, PolyFAAs, PFAA precursors, or other groups that are not described here.

Figure 9. A comprehensive overview of PFAS groups, their structural traits, examples and notes on whether corresponding common nomenclatures (including acronyms) exist.



* Strictly speaking, these substances are not fluorotelomers, as they are not derived from the telomerization process. Despite this, they are termed here "n:1 fluorotelomer-based" substances for readability. Future work may consider to identify more proper terminology for this group of PFASs.

** Note that for many compounds such as HFP and TFE, there are different synthesis routes with different starting materials, and here shows only one of them.

*** Note that there are three synthesis routes shown here for manufacturing of PFCAs, from PACFs, PFAIs and n:2 FTIs. Note that different synthesis routes may generate PFCAs with different perfluorocarbon chain lengths.

Sources: (1) Siegemund G, Schwertfeger W, Feiring A, Smart B, Behr F, Vogel H, McKusick B. *Fluorine Compounds, Organic*, 3rd ed.; Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany, 2000; Vol. 33. (2) Banks RE, Smart BE, Tatlow JC. Organofluorine Chemistry: Principles and Commercial Applications. New York: Plenum, 1994. (3) Buck RC, Franklin J, Berger U, Conder JM, Cousins IT, De Voogt P, Jensen AA, Kannan K, Mabury SA, van Leeuwen SPJ. Perfluoroalkyl and polyfluoroalkyl substances in the environment: terminology, classification, and origins. *Integr Environ Assess Manag* **2011**, 7 (4), 513–541. (4) Wang Z, Cousins IT, Scheringer M, Buck RC, Hungerbühler K. Global emission inventories for C4-C14 perfluoroalkyl carboxylic acid (PFCA) homologues from 1951 to 2030, Part I: production and emissions from quantifiable sources. *Environ Int* **2014**, *70*, 62–75. (5) Moffett RH, Howell JL, Hoerter JM, Shtarov AB, Jannerfeldt G, Johnston SB, Keenan J, Warriner C, Closser DM. *Perfluoroalkylpolyethers* in *Synthetics, Mineral Oils, and Bio-Based Lubricants: Chemistry and Technology* (third edition), Edited by Rudnick LR. 2020. CRC Press. ISBN: 978-1-138-06821-6. (6) Grot W. *Fluorinated Ionomers*. William Andrew 2011. ISBN: 978-1-437-74457-6.

Figure 10. An overview of some common synthesis routes of different individual or groups of PFASs based on publicly accessible source

Notes

[9] Note that a “saturated carbon moiety” means no unsaturated bonds occurring in the moiety, including double bond (=), triple bond (≡) or aromatic rings, and thus, a saturated carbon moiety is always considered aliphatic.

[10] According to Buck et al., fluoropolymers are “*carbon-only* polymer backbone with F directly attached to backbone C atoms”, whereas perfluoropolyethers are “*ether* polymer backbone with F atoms directly attached” (i.e. having –C–O–C– moieties on the polymer backbone).

[11] $(HO)_2(O)PO–(CH_2CH_2O)_n–CH_2CF_2–(OCF_2)_p–(OCF_2CF_2)_q–OCF_2CH_2–(OCH_2CH_2)_n–OP(O)(OH)_2$; Trier X, Granby K, Christensen JH. Polyfluorinated surfactants (PFS) in paper and board coatings for food packaging. *Environ Sci Pollut Res Int*. 2011;18(7):1108-1120. doi:10.1007/s11356-010-0439-3

[12] In Buck et al. (2011), side-chain fluorinated polymers are defined as “nonfluorinated polymer backbone with fluorinated side chains”.

Chapter 3. Practical Guidance on How to Use the PFAS Terminology

As shown above, PFASs are a chemical class with diverse molecular structures (e.g. neutral, anionic, cationic or zwitterionic; with or without aromatic rings; non-polymers or polymers; low molecular weight or high molecular weight) and thus diverse physical, chemical and biological properties (e.g. involatile or volatile; water soluble or water insoluble; reactive vs. inert; bioaccumulative or non-bioaccumulative). Therefore, it is highly recommended that such diversity be properly recognized and communicated in a clear, specific and descriptive manner. The following sections aim to provide practical guidance to governments and other stakeholders on how to use the PFAS terminology, starting from the distinction between the general definition described here and user-specific working scopes of PFASs. An overarching rationale behind the practical guidance is to use and build upon existing common terminologies such as in this report, in Buck et al. (2011) and common practices in organic chemistry as set by IUPAC and CAS, unless it is essential to deviate from existing naming conventions in order to keep the consistence and coherence of the PFAS terminology.

3.1. Distinction between the General Definition and User-Specific Working Scopes of PFASs

It should be noted that the revised definition of PFASs in Section 2.3 refers to a general definition of PFASs that is coherent and consistent across compounds based on chemical structure and is easily implementable for distinguishing between PFASs and non-PFASs, also by non-experts. It does not include any minimal or maximal chain length requirements, or any other considerations beyond chemistry. It also does not conclude that all PFASs have the same properties, uses, exposure and risks.

While this general definition of PFASs may be viewed as too broad, encompassing thousands or more compounds, for anyone to address all of them at once, it serves as a starting and reference point to guide individual users to have a comprehensive understanding of the PFAS universe and to keep the big picture of the PFAS universe in mind. At the same time, individual users may define their own PFAS working scope for a specific activity according to their specific needs by combining this general definition of PFASs with additional considerations (e.g. specific properties, use areas). For example, the US Interstate Technology & Regulatory Council (ITRC)[13] used a working scope of “C_nF_{2n+1}” ($n>2$) in making its own PFAS fact sheets. Another example is the working scope used in compiling the OECD 2018 PFAS List, namely $–C_nF_{2n}–$ ($n \geq 3$) and $–C_nF_{2n}OC_mF_{2m}–$ (n and $m \geq 1$). Also, the addition of criteria such as bioavailability and persistence in Gore Fabrics’ Goal and Roadmap[14] for Eliminating PFCs of Environmental Concern may be regarded as a way of setting working scopes.

This report does not make any recommendation on how a working scope should be set up regarding which factors to consider (which depend on specific local context)[15], nor on PFAS grouping[16]. However, when a working scope of PFASs is used, this report highly recommends that users clearly provide the context and rationale for selecting their PFAS working scope in order to provide transparency and avoid confusion by others.

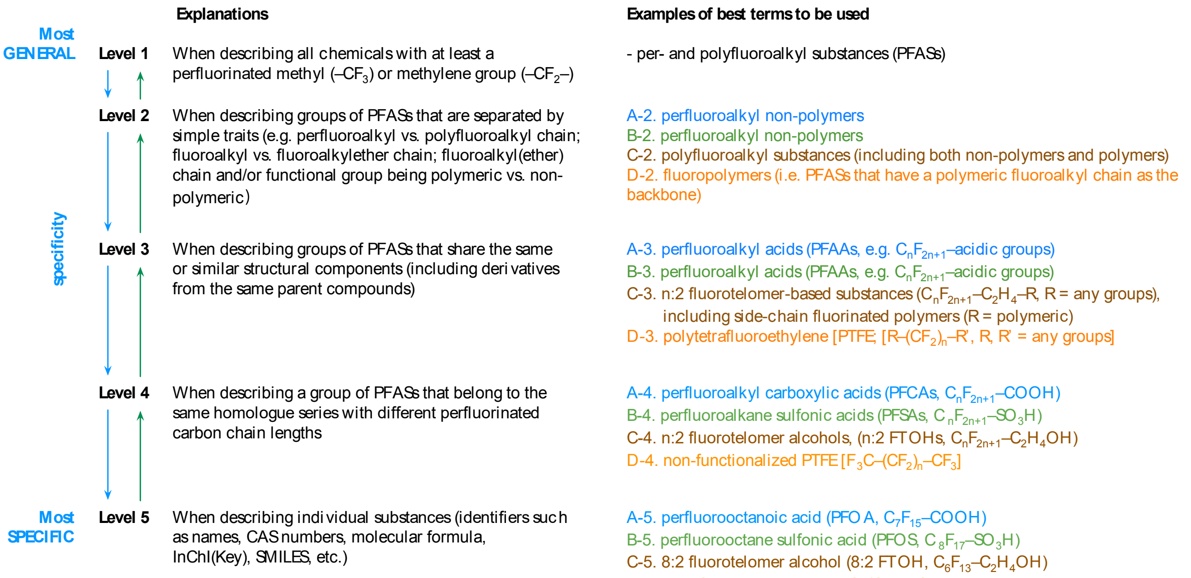
3.2. Practical guidance on how to identify and use suitable PFAS terms

The term “PFASs” does not inform whether a compound is harmful or not, but only communicates that the compounds under this term share the same trait for having a fully fluorinated methyl or methylene carbon moiety. In addition, particularly for PFASs without an assigned CAS No., a lot of parallel and often non-intuitive acronyms are employed, potentially prohibiting effective communication and creating barriers for synthesizing knowledge. This section aims to provide practical guidance on how to identify and use suitable terms to foster communication around PFASs with the aim of being accurate, precise, understandable by others, and consistent.

First, it is strongly recommended that the PFAS terminology be used in a clear, specific and descriptive manner. It should be noted that “PFASs” is a broad, general, non-specific term, which should only be used when talking about all the substances included in the PFAS definition described here (or the user should clearly define the scope of which substances are being referred to as PFASs in the documents they prepare). Otherwise, it would introduce ambiguity and even factual error in the statements (as occurred sometimes in past literature). For example, not all PFASs are surfactants, and thus, a statement “PFASs are surfactants” is factually inaccurate. Table 1 highlights examples of ambiguous statements, which when are overgeneralized may lead to ambiguity, and factual inaccuracies and miscommunication in some cases. Therefore, it is recommended that users always ask the following two questions when drafting a statement: (1) Am I referring to all PFASs or not? (2) If not, what term(s) would mostly clearly describe the substance(s) that my statement is referring to? There could be multiple ways by users to locate the right levels of terms that are clear, specific and descriptive for specific statements, by combining and ordering traits such as polymeric vs. non-polymeric, PFAAs vs. PFAA precursors, or side-chain fluorinated polymers vs. fluoropolymers vs. perfluoropolyethers. Figure 11 shows different levels of PFAS terms and their respective characteristics in terms of clarity and specificity, along with examples; one may either start from Level 1 (most general) and move downwards (with the question of whether it is specific enough), or Level 5 (most specific) and move upwards (with the question of whether it can be further generalized), to locate the right level of terms for a specific statement. Table 1 also includes examples of good practice to refine ambiguous statements using more suitable terms. Furthermore, individual PFASs need to be named in a clear, specific and descriptive manner.

Table 1. Examples of ambiguous statements and associated good practices of using more specific PFAS terminology to refine these statements

<u>Examples</u> of ambiguous statements (which may also result in factual inaccuracy in some cases)	**<u>Examples</u> of good practices of using the PFAS terminology to avoid errors and reduce ambiguity**	
	(1) Using more specific PFAS terms	**(2) Adding qualifiers (less favorable than (1), as it remains quite ambiguous)**
<u>PFASs</u> were investigated in human milk.	**C_4–C_{14} PFCAs** were investigated in human milk.	**15 non-polymeric** PFASs were investigated in human milk.
<u>PFASs</u> are used to make protective coatings on common household products.	**Fluorotelomer-based side-chain fluorinated polymers** are used to make protective coatings on common household products.	**A number of polymeric** PFASs are used to make protective coatings on common household products.
<u>PFASs</u> are relatively ubiquitous in the environment at low concentrations. (factually inaccurate)	**PFCAs** are relatively ubiquitous in the environment at low concentrations.	**A number of** PFASs are relatively ubiquitous in the environment at low concentrations.
<u>PFASs</u> are water repellent, oil, grease and dirt repellent surfactants. (factually inaccurate)	**Many perfluorooctane sulfonyl fluoride-based derivatives** are water-, as well as oil-, grease- and dirt-repellent surfactants.	**A number of** PFASs are water-, as well as oil-, grease- and dirt-repellent surfactants.



		Explanations	**Examples of best terms to be used**
Most GENERAL	**Level 1**	When describing all chemicals with at least a perfluorinated methyl ($–CF_3$) or methylene group ($–CF_2–$)	- per- and polyfluoroalkyl substances (PFASs)
	Level 2	When describing groups of PFASs that are separated by simple traits (e.g. perfluoroalkyl vs. polyfluoroalkyl chain; fluoroalkyl vs. fluoroalkylether chain; fluoroalkyl(ether) chain and/or functional group being polymeric vs. non-polymeric)	A-2. perfluoroalkyl non-polymers B-2. perfluoroalkyl non-polymers C-2. polyfluoroalkyl substances (including both non-polymers and polymers) D-2. fluoropolymers (i.e. PFASs that have a polymeric fluoroalkyl chain as the backbone)
	Level 3	When describing groups of PFASs that share the same or similar structural components (including derivatives from the same parent compounds)	A-3. perfluoroalkyl acids (PFAAs, e.g. C_nF_{2n+1}–acidic groups) B-3. perfluoroalkyl acids (PFAAs, e.g. C_nF_{2n+1}–acidic groups) C-3. n:2 fluorotelomer-based substances ($C_nF_{2n+1}–C_2H_4–R$, R = any groups), including side-chain fluorinated polymers (R = polymeric) D-3. polytetrafluoroethylene [PTFE; $[R–(CF_2)_n–R'$, R, R' = any groups]
	Level 4	When describing a group of PFASs that belong to the same homologue series with different perfluorinated carbon chain lengths	A-4. perfluoroalkyl carboxylic acids (PFCAs, $C_nF_{2n+1}–COOH$) B-4. perfluoroalkane sulfonic acids (PFSAs, $C_nF_{2n+1}–SO_3H$) C-4. n:2 fluorotelomer alcohols, (n:2 FTOHs, $C_nF_{2n+1}–C_2H_4OH$) D-4. non-functionalized PTFE [$F_3C–(CF_2)_n–CF_3$]
Most SPECIFIC	**Level 5**	When describing individual substances (identifiers such as names, CAS numbers, molecular formula, InChI(Key), SMILES, etc.)	A-5. perfluorooctanoic acid (PFOA, $C_7F_{15}–COOH$) B-5. perfluorooctane sulfonic acid (PFOS, $C_8F_{17}–SO_3H$) C-5. 8:2 fluorotelomer alcohol (8:2 FTOH, $C_6F_{13}–C_2H_4OH$) D-5. specific PTFE products [$F_3C–(CF_2)_n–CF_3$; X<n<Y; X,Y = integers]

Figure 11. A visual guide to identify the best terms to use for a specific statement with four examples (increasing level of specificity illustrated with same colour within examples).

Second, if users are not sure about how to name a specific compound, it is recommended to first check whether a common nomenclature (including a common acronym) already exists, e.g., in Buck et al. (2011), Barzen-Hanson et al. (2017)[17], this report and other studies, before creating their own naming conventions. For example, for CAS No. 678-39-7, a common name “8:2 fluorotelomer alcohol” and a common acronym “8:2 FTOH” already exist, and should be used instead of other synonyms.

Third, acronyms are often necessary in communicating PFASs to avoid writing very long names all the time; however, the same acronym may refer to different full names or different forms of the same substance (e.g. the parent acid, the anion form, and various salt forms), depending on context and personal understanding. To avoid confusion, it is recommended that acronyms be spelled out when being mentioned for the first time in the text and used consistently throughout the text.

Fourth, while chemical names and associated acronyms are the most common chemical identifiers being used, it is also recommended that other more specific identifiers such as CAS No., SMILES (simplified molecular input line entry specification), InChI (international chemical identifier), InChIkey (a hashed version of the full InChI) and/or structural formula[18] are provided for possibilities of cross-checking. This may also be useful in reporting the chemical identities of PFASs that have been registered as substances of unknown or variable composition, complex reaction products, or biological materials (UVCBs, e.g., CAS No. 69991-67-9 = 1-propene, 1,1,2,3,3,3-hexafluoro-oxidized, polymd.)[8].

Notes

[13] The latest version of the fact sheet on naming conventions of PFASs is from April 2020: https://pfas-1.itrcweb.org/fact_sheets_page/PFAS_Fact_Sheet_Naming_Conventions_April2020.pdf

[14] Here it refers to the version published on January 31, 2017, which can be found at: https://drive.google.com/file/d/0BxvQ_I44P_9eeTlwYUJCekhLNlE/view

[15] Future work compiling various existing practices of defining working scope under different context may be beneficial to provide further guidance to governments and other stakeholders on this matter.

[16] In a recent scientific article, various grouping strategies for PFASs were reviewed and the motivations, advantages and disadvantages for each approach were discussed; for more details, see Cousins et al. 2020. *Environmental Science: Processes & Impacts*, 22, 1444–1460, https://doi.org/10.1039/D0EM00147C

[17] In the Supporting Information, Barzen-Hanson et al. developed a simplified, manual IUPAC-based naming system for the PFASs that they identified in their non-target screening. For more details, see Barzen-Hanson et al. 2017. *Environmental Science & Technology*. 51(4), 2047–2057. https://doi.org/10.1021/acs.est.6b05843

[18] These identifiers may be found and verified using online databases, such as the CAS Common Chemistry (https://commonchemistry.cas.org), ChemSpider (http://www.chemspider.com), NORMAN Suspect List Exchange (https://www.norman-network.com/?q=suspect-list-exchange), OECD eChemPortal (https://www.echemportal.org/echemportal/), PubChem (https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101), SciFinder (http://scifinder.cas.org) and US EPA CompTox Chemicals Dashboard (https://comptox.epa.gov/dashboard/chemical_lists/PFASOECD).

Chapter 4. Systematic characterization and categorization of PFASs

As users often define their own working scope of PFASs according to their specific needs (see Section 3.1), they need to characterize PFASs based on molecular structures (and other considerations) and then categorize them by comparing characterization traits against specific needs (e.g. whether a compound falls or does not fall into their working scope). For example, the recent listing of PFOA and PFOA-related compounds under the Stockholm Convention requires regulators across the world to be able to identify PFOA-related compounds from a pool of PFASs.

However, given the high complexity and diversity of PFASs, it can be a challenging task to characterize and categorize PFASs based on their chemical structures in a coherent and consistent manner, particularly for non-experts. Detailed challenges may include needs of specialized chemistry knowledge (e.g. on transformation), different interpretations of structural traits by users for different groups of PFASs, and potential for human errors including oversights and typing errors (Sha et al. 2019). In addition, different users may have very different needs, and there is no single categorization/grouping system that can meet all needs.

Therefore, this section provides a standardized system for systematic characterization of different PFASs based on molecular structural traits that will allow stakeholders to make their own categorization in a coherent and consistent manner. Molecular structure-based elements of such a characterization system are provided in Table 2, with some examples of applications given in Table 3. For example, if someone would like to have the grouping of linear PFCAs, they would just need to search for molecules with the right characterization traits as defined in Table 3: under “fluorinated carbon chain (A)”, having “alkyl”, “perfluoro”, “linear”, “saturated”, “non-polymeric”; under “functional group B”, having “COOH” and “non-polymeric”; and under “stoichiometry between A and B”, having “1:1”. The system is flexible for future refinement including possible addition of new elements as needed and also applications to new groups of PFASs as identified.

In addition to manual application of the system to characterize and categorize PFASs, the elements presented here may also be used as inputs for developing cheminformatic tools that would allow automatized characterization and categorization of PFASs, as demonstrated in Sha et al. (2019).

In that study, an algorithm was developed to systematically parse a PFAS molecule into three fragments namely C_nF_{2n+1}–X–R, where C_nF_{2n+1}– refers to the fluorinated carbon moiety and –X–R refers to functional group moiety. X was used to identify whether a PFAS molecule falls into the target group of perfluoroalkane sulfonyl fluoride-derivatives (where X = SO_2), perfluoroalkanoyl fluoride derivatives (where X = CO), n:1 fluorotelomer-based compounds (where X = CH_2 and R does not have a CH_2 or CH moiety connecting with X), or n:2 fluorotelomer-based compounds (where X = CH_2CH_2). The algorithm was applied to a set of 770 PFASs from the OECD 2018 PFAS List and identified PFASs from the target four groups as intended. The algorithm was also able to identify PFASs that were mis-categorized in the OECD 2018 PFAS List, as the original categorization was done manually.

The algorithm developed in Sha et al. (2019) serves as a proof-of-concept, and thus has its limitations in terms of its purpose (i.e. to identify whether a PFAS falls into one of the four target groups) and function (e.g. it cannot handle PFASs with more than one functional group moieties). However, it shows the potential of such cheminformatics approaches, which can be expanded using the elements provided here for systematic characterization and categorization of PFASs in a coherent and consist manner, particularly for non-PFAS experts. It needs to be noted that tools proposed here that integrate the concept presented in Sha et al. (2019) and the proposed elements of a characterization system is one way of developing cheminformatics-based tools for systematic characterization and categorization of PFASs. Depending on the needs, there may also be other ways of doing so, including adding other elements into consideration (e.g. a ToxPrints approach that also considers structures related to adverse outcomes[19]) or implementing in other ways (e.g. using Markush structures to annotate existing lists[20]). An outlook of future developments is provided in the next section.

Table 2. Molecular structure-based elements of a characterization system for PFASs.

PFASs may be parsed into the following two structural parts	**Molecular structure-based elements to be considered**	**Note**
Fluorinated carbon chain (A)	alkyl vs. alkylether	Whether the fluorinated carbon chain is carbon only or has oxygen-linkage(s) between fluorinated carbons e.g., $–C_nF_{2n}–$ vs. $–C_nF_{2n}–O–C_mF_{2m}–$
	perfluoro vs. polyfluoro	Whether all hydrogen on the fluorinated carbon chain are replaced by fluorine (i.e. perfluoro) or not (i.e. polyfluoro) e.g., $H–C_2F_4–$, $Cl–C_2F_4–$, $CF_3CF_2–C_2H_4–C_2F_4–C_2H_4–$, $CF_3CF_2–CH_2–CF_2–CH_2–CF_2–$, etc. = polyfluoro
	linear vs. branched vs. cyclic	Whether the fluorinated carbon chain is linear, branched or cyclic e.g., $–C_6F_{13}$ vs. $–C_3F_6CF(CF_3)_2$ vs. –cyclo(C_6F_{12})
	saturated vs. non-saturated	Whether there is any unsaturated bond (a double or triple bond) in the fluorinated carbon chain e.g., $–CF_2CF_2$- vs. $–CF=CF–$
	polymeric vs. non-polymeric	Whether the fluorinated carbon chain is polymeric or non-polymeric e.g. using the OECD definition (http://www.oecd.org/env/ehs/oecddefinitionofpolymer.htm) [Note: this may require additional consideration, e.g. whether a minimum perfluorocarbon moiety chain length of 20 would be required][21]
	chain length of the fluorinated carbon chain	e.g., for perfluoroalkylether-based substances, the total length of perfluoroalkylether moieties including both carbon and oxygen atoms will be counted, and additional information on the number of oxygen atoms will be provided as supplementary information, similarly to what is in the OECD 2018 list.

Functional group (B)	types and structures of functional groups	As there is no common classification system of functional groups, here a simplified scheme is proposed that is intended to distinguish those reactive and non-reactive (or those not so reactive) groups under natural conditions, which can be used to differentiate e.g. PFAAs and PFAA precursors. 1. Non-reactive groups (or those not so reactive) 1.1. H, Cl, Br 1.2. N, P 1.3. COOH 1.4. SO_3H 1.5. PO_3H_2 2. Reactive groups 2.1. I 2.2. SO_2H – sulfinic acids 2.3. PO_2H 2.4. CH_2–R – possibly n:1 fluorotelomers 2.5. CH_2CH_2–R – possibly n:2 fluorotelomers 2.6. CO–R (other than COOH) – alkanoyl fluoride-derivatives 2.7. SO_2–R (other than SO_2OH) – sulfonyl fluoride-derivatives 2.8. C_mH_{2m+1}, OC_mH_{2m+1}, C_mH_{2m-1} 3. Others (which may be refined in future work)
	polymeric vs. non-polymeric	Whether the non-fluorinated functional group is polymeric or non-polymeric, e.g. using the OECD definition (http://www.oecd.org/env/ehs/oecddefinitionofpolymer.htm) [Note: this may require additional consideration of additional qualifier, e.g. whether a minimum chain length of 20 would be required]
stoichiometry between A and B	How are fluorinated carbon chain(s) connected with non-fluorinated carbon chain(s)/functional groups?	1:0 = no functional group
		1:1/1:2/1:3 = one fluorinated carbon chain connected with 1/2/3 functional group(s)
		2:1 = two fluorinated carbon chains connected with one functional group, e.g. PFPIAs

Table 3. Examples using the proposed characterization system.

	Possible elements to be considered	**Example 1: Linear PFCAs**	**Example 2: PFOA precursors**	**Example 3: ADONA**	**Example 4: 6:2 FT-acrylate polymer**	**Example 5: PTFE with –COOH on each end**
Fluorinated carbon chain (A)	alkyl vs. alkylether	Alkyl	Alkyl	Alkylether	Alkyl	Alkyl
	perfluoro vs. polyfluoro	Perfluoro	Perfluoro	Polyfluoro	Perfluoro	Perfluoro
	linear vs. branched vs. cyclic	Linear	Linear + Branched	Linear	Linear	Linear
	saturated vs. non-saturated	Saturated	Saturated	Saturated	Saturated	Saturated
	polymeric vs. non-polymeric	Non-polymeric	Non-polymeric	Non-polymeric	Non-polymeric	Polymeric
	chain length	1–20	>=7 (in the case of when A and B connects via a carbon atom); >=8 (in the case of when A and B connects via other atoms other than a carbon atom)	6 + 2O	6	XX
Non-fluorinated functional group (B)	types and structures of functional groups	1.3 COOH	2 Reactive groups	1.3 COOH	2.5 CH_2CH_2–R – possibly n:2 fluorotelomers	1.3 COOH
	polymeric vs. non-polymeric	Non-polymeric	Non-polymeric; polymeric	Non-polymeric	Polymeric	Non-polymeric
Connection between A and B	How are fluorinated carbon chain(s) connected with non-fluorinated carbon chain(s)?	1:1	1:1	1:1	n:1	1:2

Notes

[19] For an example, see https://figshare.com/articles/presentation/PFAS_Toxprints_A_Hierarchical_Structure-Based_Categorization_Method_for_Characterization_of_Per-_and_Polyfluoroalkyl_Substances/12834329. Currently, the US EPA is preparing a manuscript on this approach, including means for applying it.

[20] A Markush structure is a generic type of description of chemicals used to summarize a potentially very large set of closely related chemicals in a single condensed representation. It may consist of a “core” chemical structure and a list of possible substituents attached to it, with four substituent options: substituent variation (allowing different substituents at a position), position variation (allowing different attachment points for a substituent), frequency variation (allowing substituents to occur multiple times) and homology variation (using generic expressions covering many specific substituents like “alkyl”). For more details, see, e.g., Geyer P. 2013. *World Patent Information*, 35(3), 178–182, https://doi.org/10.1016/j.wpi.2013.05.022.

The US EPA CompTox Chemicals Dashboard uses “Markush structures” to organize its PFAS list. In brief, the Dashboard has curated 112 PFAS Markush structures with unique DTXSIDs assigned (e.g. DTXSID80893896 $HOOC–(CF_2)_n–COOH$ for perfluoroalkyl (linear) dicarboxylic acids, i.e. homology variation). Each PFAS Markush structure is considered a generalized substance or “parent ID” that can be associated with one or many “child IDs” within the Dashboard (e.g. DTXSID80893896 are linked to 12 linear perfluoroalkyl dicarboxylic acids with different fluorinated carbon chain lengths in the Dashboard). For more details, see https://comptox.epa.gov/dashboard/chemical_lists/EPAPFASCAT.

[21] In many jurisdictions, a polymer is defined as a substance that has over 50 percent of the weight consisting of polymer molecules and the amount of polymer molecules presenting the same molecular weight must be less than 50 weight percent of the substance. A polymer molecule is defined as a molecule that contains a sequence of at least 3 monomer units, which are covalently bound to at least one other monomer unit or other reactant. Thus, a mixture of 8:2, 10:2 and 12:2 fluorotelomers (each 33%) can theoretically be regarded as a polymer.

Chapter 5. Areas for Future Work

While this report makes advancement on several important points regarding the PFAS terminology and practical guidance of how to use the PFAS terminology, it also recognizes that the following four areas warrant further work within the field of PFASs (i.e. areas one and two) and beyond (i.e. areas three and four), in order to facilitate clear and unambiguous communication of PFASs.

First, a centralized PFAS nomenclature database/platform may be considered. With the further advancement and application of non-target screening methods, many more unknown PFASs are expected to be discovered in the future. Such a centralized nomenclature database/platform can help foster the use of harmonized names and acronyms for the same compounds. It can also help to link different common names and acronyms that have been used over time to specific substances.

Second, further development of cheminformatics-based tools for automated systematic characterizing and categorizing PFASs would advance the field. A solely structure-based approach proposed in the report (i.e. Chapter 4) may serve as one starting point for possible joint development of an open source tool by experts from different online databases/platforms so that such a tool may be compatible for different online databases/platforms. In addition, as cheminformatics is a fast-developing field, future work may be conducted to monitor, assess and communicate which cheminformatics tools are developed for which purposes.

Third, further work on the characterization and reporting of polymers should be considered, as well as assessment of their properties. The current definitions of polymers in many jurisdictions originate from the OECD definition of polymer that was developed in the early 1990s, and in some cases, substances containing a significant fraction of low-molecular-weight molecules may be identified as polymers, as indicated in Footnote 21. This may impact how individual substances are registered (or not registered) and subsequent regulatory requirements of safety information. Thus, chemical compositions in substances that are identified as polymers may warrant a closer look, particularly in terms of their low-molecular-weight content, based on lessons learned in the past three decades. In addition, the current reporting of many polymers are often rather ambiguous (e.g. a polymer may be named as a co-polymer of three monomers A, B and C without indicating how the monomers are connected and in which molecular ratios, reaction schemes and molecular weight range of individual compositions, which could have implications on assessing the fate, behavior and risks of specific polymer products). Thus, future international efforts are needed to look into ways to improve the understanding of polymer structures including access to necessary information, focusing on polymeric PFASs or on polymers in general.

Fourth, as shown in Figure 8, there are many groups of organofluorine substances other than PFASs. Future work could also look into these compounds, including the terminology of many fluorinated aromatics.

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This report summarizes recent efforts by the OECD/UNEP Global PFC Group in reviewing the universe and terminology of per- and polyfluoroalkyl substances (PFASs) to provide recommendations and practical guidance to all stakeholders with regard to the terminology of PFASs.

In particular, this report highlights a revised PFAS definition to comprehensively reflect the universe of PFASs, practical guidance on how to use the PFAS terminology, a systematic approach to characterization of PFASs based on molecular structural traits to assist stakeholders, including non-experts, in making their own categorization based on their needs, and areas in relation to the PFAS terminology that warrant further development.

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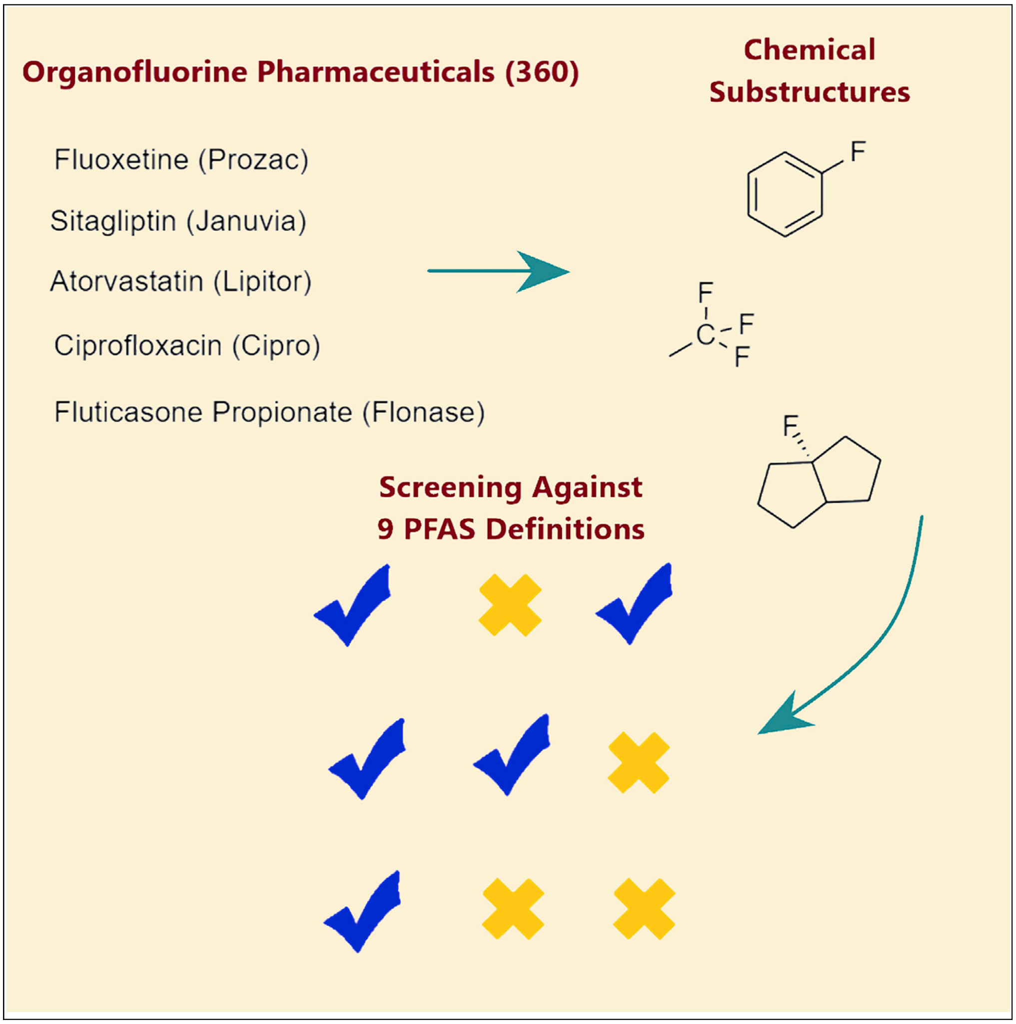
Implications of PFAS definitions using fluorinated pharmaceuticals



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Highlights

Nine PFAS definitions were evaluated and used to screen 360 organofluorine drugs

Broad definitions include many top prescribed pharmaceuticals, e.g., Prozac and Lipitor

Implications for fluorinated pharmaceuticals depend on intended use of the definition

Findings necessitate discussion of possible exemptions for pharmaceuticals

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Implications of PFAS definitions using fluorinated pharmaceuticals

Emily Hammel,[1,3,*] Thomas F. Webster,[1] Rich Gurney,[2] and Wendy Heiger-Bernays[1]

SUMMARY

There are 9,000+ per- and polyfluoroalkyl substances (PFAS) in existence, which makes studying and regulating PFAS individually, or even as small mixtures, infeasible. Multiple PFAS definitions based on structure have been proposed, yet these definitions do not consider the implications for the full suite of organofluorine chemicals. For example, organofluorine pharmaceuticals, whose use may be essential and are found in human serum and wastewater, are not uniformly identified across all definitions. Using nine definitions prepared by various stakeholders, we screened the 360 organofluorine pharmaceuticals approved and used globally between 1954 and 2021. Definitions ranged in their inclusion of organofluorine pharmaceuticals (1%–100%). The most inclusive definitions include several top prescribed pharmaceuticals, e.g., Prozac and Lipitor. This analysis provides a framework against which organizations can make decisions about how best to proceed when defining PFAS.

INTRODUCTION

Since manufacturing began in the 1940s, per- and poly-fluoroalkyl substances (PFAS) have been widely used in textile manufacturing, food packaging, cookware, pesticide applicators, medical equipment, and other commercial products (Glüge et al., 2020). To date, upward of 9,000 PFAS have been identified (USEPA, 2021a). Many are toxic, persistent, and widely detected in the environment and human serum, prompting global discussion around their cost and benefits (Cordner et al., 2021), essential uses (Cousins et al., 2019), and effective strategies for regulation.

The large number of PFAS and the substitution of legacy compounds such as PFOA and PFOS by newer compounds—about which less is known although they may turn out to be just as problematic—has prompted movement away from the traditional chemical-by-chemical regulation toward regulation of these compounds as a class in both the U.S. (116th Congress, 2019; Kwiatkowski et al., 2020; Bălan et al., 2021) and Europe (ECHA, 2021). Several agencies, non-governmental organizations, and other groups have adopted class-based PFAS definitions for regulatory and non-regulatory purposes (Tables 1 and 2). Notably, the U.S. National Defense Authorization Act (NDAA) includes the PFAS Act of 2019, which adopts a structural definition classifying PFAS as any compound with at least ''one fully fluorinated carbon'' (116th Congress, 2019). The act authorizes funding for Department of Defense (DoD) initiatives related to PFAS remediation in areas impacted by military activities and sets restrictions on the use of PFAS in firefighting foam, personal protective equipment for firefighters, and food packaging used in military meals. Importantly, the act also sets requirements for environmental monitoring for PFAS in surface and groundwater and biomonitoring for PFAS among military personnel.

Recent work describes the advantages and disadvantages of different grouping strategies of PFAS based on their persistence and toxicity (Cousins et al., 2020; Wallington et al., 2021), yet relatively little work has been done to understand the differences between specific PFAS definitions and what set of compounds they will include. We focus here on organofluorine pharmaceuticals: they present an opportunity to assess the implications of PFAS definitions for a diverse but well-defined set of chemicals used globally. Organic fluorine was first introduced to the pharmaceutical industry in 1954 and is useful in altering the physiochemical properties of a drug to achieve a desired pharmacological effect (Inoue et tl., 2020). Pharmaceuticals represent a class of regulated chemicals whose use might be deemed at least partially ''essential'' for medical purposes. They are also of interest to environmental scientists for a number of reasons. For example, pharmaceutical waste enters the wastewater treatment systems (Kolpin et al., 2002), where metabolites are

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Table 1. Organizations, proposed and adopted definitions of PFAS, listed by year, evaluated in this analysis

Organization	Year	Regulatory?	Intended purpose
Buck et al.	2011	No	Establish clarity around the nomenclature of PFAS, including classifications based on molecular structure
OECD	2018, 2021	No	Characterize the universe of PFAS based on structural similarities between compounds containing fully fluorinated methyl or methylene moieties
Glüge et al.	2020	No	Understand major use areas; support work being done to address essentiality and feasibility of PFAS-free replacements
TURA Program, Massachusetts	2021a, 2021b	Yes	Establish new toxic substance category on toxic use inventory list in Massachusetts
U.S. EPA OPPT	2021	Yes	Lists chemicals for review under the Toxic Substances Control Act (TSCA) to evaluate risks to human health and the environment
NDAA, WA, CA, VT, ME[a] "≥1 Fully Fluorinated Carbon"	2019, 2020, 2021	Yes	Applications vary across agencies; reporting of PFAS in media impacted by military activities, ban of PFAS used in firefighting foam and equipment, and biomonitoring of PFAS in military personnel (NDAA); reporting and eventual ban of PFAS used in firefighting foam and firefighting equipment (CA); firefighting foam and food contact materials (WA); firefighting foam and products used in rugs/carpets/food packaging/ski wax (VT); any product containing intentionally added PFAS (ME).
NGOs[b] "All Organofluorine"	2021	No	Environmental advocacy; reflects organizations' broader mandates to protect constituents and the environment

[a] Authorities whose legislation defines PFAS as a class of fluorinated organic chemicals containing at least one fully fluorinated carbon atom.

[b] NGOs that advocate for broader definitions of PFAS to include all organofluorines.

either discharged back into the receiving waters, or are found in the biosolids after treatment (Massey and Waldron, 2011). While the degradation products of many pharmaceuticals remain unknown, active pharmaceutical ingredients and their metabolites are measurable in wastewater effluent (Yu et al., 2006). Models to predict biodegradability suggest some organofluorine pharmaceuticals may degrade into metabolites with trifluoromethyl groups and thus are likely to persist in the environment given the strength and durability of the CF_3-R functional group (Neuwoehner et al., 2009).

Definitions of PFAS are developed for multiple purposes, also referred to as "working scopes" (OECD, 2021), and can be both regulatory and non-regulatory. Regardless of its intended purpose, a useful definition requires clear, unambiguous language that is interpretable by stakeholders. In this analysis, we describe nine definitions of PFAS and examine some potential ambiguities in their language. We use each definition to screen a comprehensive list of organofluorine pharmaceuticals to determine which pharmaceuticals are included. Finally, we discuss some implications of these definitions given their intended purpose for use in regulatory or non-regulatory initiatives. Similar analyses could be performed for other groups of compounds.

RESULTS

Definitions of PFAS and their intended uses

Tables 1 and 2 show the nine PFAS definitions and their intended purpose. These include definitions developed by Buck et al. (2011), the Organisation for Economic Co-operation and Development (OECD), Glüge et al. (2020), the Toxic Use Reduction Act (TURA) Program of Massachusetts, U.S. EPA Office of Pollution Prevention and Toxics (U.S. EPA OPPT) (USEPA, 2021b), the NDAA (116th Congress, 2019) and laws from the states of Washington (2021), Vermont (2021), Maine (2021), and California (2020), and several non-governmental environmental advocacy organizations (e.g., Sierra Club of Massachusetts)

Table 2. Definitions of PFAS included in analysis

Definition	Formal definition verbatim from organization	Informal interpretation
Buck et al. (2011)	"Aliphatic substances containing one or more C atoms on which all the H substituents present in the nonfluorinated analogues from which they are notionally derived have been replaced by F atoms, in such a manner that PFASs contain the perfluoroalkyl moiety C_nF_{2n+1}–."	Compounds that contain at least one carbon atom that is bound to three fluorine atoms (-CF_3). The structure must be saturated with no double or triple bonds (the only definition with this restriction).
OECD (2018)	"PFASs, including perfluorocarbons, that contain a perfluoroalkyl moiety with three or more carbons (i.e. –C_nF_{2n}–, $n \geq 3$) or a perfluoroalkylether moiety with two or more carbons (i.e. –$C_nF_{2n}OC_mF_{2m}$–, n and $m \geq 1$)."	Compounds with at least three carbons on which all of the hydrogens have been replaced by a fluorine atom, so as to form a three-carbon unit with the subunits of (-CF_2-). It also includes compounds with an oxygen placed between two carbon atoms on which all of the hydrogens have been replaced by a fluorine atom, so as to form a carbon-oxygen-carbon unit with the subunits (-CF_2OCF_2-)
OECD (2021)	"PFASs are defined as fluorinated substances that contain at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it), i.e. with a few noted exceptions, any chemical with at least a perfluorinated methyl group (–CF_3) or a perfluorinated methylene group (–CF_2–) is a PFAS."	Compounds containing at least one carbon that has three fluorine atoms attached (–CF_3). Also includes compounds that have at least one carbon attached to two fluorine atoms (-CF_2-). In both cases, the carbon atom cannot be attached to a hydrogen, chlorine, or bromine atom. It still includes compounds whose carbon-fluorine units are attached together by an oxygen (-CF_2OCF_2-). These structures can contain rings or be arranged in a chain
Glüge et al. (2020)	In addition to substances containing C_nF_{2n+1}, where $n \geq 1$, it also "includes (i) substances where a perfluorocarbon chain is connected with functional groups on both ends, (ii) aromatic substances that have perfluoroalkyl moieties on the side chains, and (iii) fluorinated cycloaliphatic substances. Additionally, "polymeric PFAS with the –CF_2– moiety and non-polymeric PFAS with the –CF_2–CF_2– moiety … [excluding] non-polymeric substances that only contain a –CF_3 or –CF_2– moiety, with the exception of perfluoroalkylethers and per- and polyfluoroalkylether-based substances. For these two PFAS groups, substances with a –CF_2OCF_2– or –$CF_2OCFHCF_2$– moiety are also included."	Does not include compounds with a single –CF_2– or –CF_3, but can include compounds with two or more –CF_2– or –CF_3 groups. Compounds can contain rings or be arranged in a chain. Also includes compounds that contain two carbon atoms next to each other, each containing at least two fluorine atoms (–CF_2–CF_2–). The two fluorinated carbons can be attached together by an oxygen atom (–CF_2OCF_2– or –$CF_2OCFHCF_2$–).
TURA (2021a)	"Those PFAS that contain a perfluoroalkyl moiety with three or more carbons (e.g., –C_nF_{2n}–, $n \geq 3$; or CF_3–C_nF_{2n}–, $n \geq 2$) or a perfluoroalkylether moiety with two or more carbons (e.g., –$C_nF_{2n}OC_mF_{2m}$– or –$C_nF_{2n}OC_mF_m$–, n and $m \geq 1$)."	Key to this definition is that the compound must contain a string of at least three carbon atoms, each containing two or more fluorine atoms. Perfluoroalkylethers are compounds that contain two –CF_2– groups connected by an oxygen. Includes linear, branched, cyclic compounds and aromatic rings
TURA (2021b)	"Certain PFAS not otherwise listed includes those PFAS that contain a perfluoroalkyl moiety with three or more carbons (e.g., –C_nF_{2n}–, $n \geq 3$; or CF_3–C_nF_{2n}–, $n \geq 2$) or a perfluoroalkylether moiety with two or more carbons (e.g., –$C_nF_{2n}OC_mF_{2m}$– or –$C_nF_{2n}OC_mF_m$, n and $m \geq 1$), wherein for the example structures shown the dash (–) is not a bond to a hydrogen and may represent a straight or branched structure, that are not otherwise listed."	Clarifies that in TURA 2021a the (–) does not include a bond to hydrogen
U.S. EPA OPPT (2021)	"… a structure that contains the unit R-CF_2-CF(R′) (R″), where R, R′, and R″ do not equal "H" and the carbon-carbon bond is saturated (note: branching, heteroatoms, and cyclic structures are included)."	Compounds that contain a string of two adjacent carbon atoms, with one of them containing at least two fluorine atoms and the other containing at least one fluorine atom, and neither carbon bound to a hydrogen

(*Continued on next page*)

Table 2. *Continued*

Definition	Formal definition verbatim from organization	Informal interpretation
≥1 Fully Fluorinated Carbon[a]	Organic chemicals containing "at least one fully fluorinated carbon atom."	A compound with at least one carbon on which all of the hydrogen atoms have been replaced by fluorine atoms. The number of bonds on the carbon is not specified
All Organofluorine[b]	All organic compounds containing at least one fluorine atom should be classified as PFAS.	Any compound whose structure contains a carbon attached to a fluorine atom

[a] Authorities whose legislation defines PFAS as a class of fluorinated organic chemicals containing at least one fully fluorinated carbon atom (WA, VT, ME, CA, NDAA).

[b] NGOs that advocate for broader definitions of PFAS to include all organofluorines.

(Massachusetts Executive Office of Energy and Environmental Affairs, 2021). We consider two definitions proposed by the OECD, one from 2018 (OECD, 2018) and the update in 2021 (OECD, 2021). We also evaluated two definitions proposed by the TURA Program Administrative Council to the Massachusetts Department of Environmental Protection (MassDEP): the original definition developed by the TURA Science Advisory Board, represented as TURA (2021a) (Administrative Council on Toxics Use Reduction, 2021a), and an amended version clarifying the definition, represented by TURA 2021b (Administrative Council on Toxics Use Reduction, 2021b).

Screening organofluorine pharmaceuticals

Using the publicly available KEGG drug database (KEGG, 2021), 363 pharmaceuticals approved in the U.S., Japan, and Europe are identified including two over-the-counter drugs. Three compounds were excluded from analysis: the insecticide novaluron, the veterinary pharmaceutical dirlotapide, and sulfur hexafluoride (Lumason) which does not contain organically bound fluorine. The remaining 360 pharmaceuticals were included in the analysis: the complete list of chemical structures, therapeutic use areas, chemical identifiers, and numbers of prescriptions (where available) are provided in the supplemental information (Data S1).

Organofluorine pharmaceuticals can be organized by substructures within the compound. Figure 1 presents the frequency of substructures identified among the 360 fluorinated pharmaceuticals; 50% of organofluorine pharmaceuticals contain a single fluorine; 35% contain a single aromatic fluorine; 10% contain more than three fluorine atoms. Only four pharmaceuticals were fully or nearly fully fluorinated aliphatic compounds. There were 88 compounds containing at least one trifluoromethyl moiety (R-CF_3) where R is not hydrogen, 15 of which contained two trifluoromethyl moieties.

Table 3 summarizes the proportion of organofluorine pharmaceuticals that meet each of the nine structural definitions, disregarding for now their intended applications. The most inclusive is the "all-organofluorine" definition, including 100% of organofluorine pharmaceuticals. The revised TURA 2021b definition is least inclusive and captures the fewest (1.1%). We will now discuss each PFAS definition in roughly in the order in which they were proposed.

PFAS identified by Buck et al.

Buck et al. (2011) provided one of the earliest and most widely used of the PFAS definitions, replacing earlier terminology. According to Buck et al., PFAS are "aliphatic substances containing one or more C atoms on which all the H substituents present in the nonfluorinated analogs from which they are notionally derived have been replaced by F atoms, in such a manner that PFASs contain the perfluoroalkyl moiety C_nF_{2n+1}–." A restatement in less technical language is given in Table 2. Importantly, this definition excludes aromatic compounds (structures containing unsaturated hydrocarbon rings with double and single bonds). Based on this definition, 8 (2.2%) fluorinated pharmaceuticals would be classified as PFAS. An example of a fluorinated pharmaceutical compound meeting the definition outlined by Buck et al. is perflubron, a contrast imaging agent previously used in magnetic resonance imaging (MRI) scans which is now being investigated as liquid oxygen used to stabilize hemorrhage during major surgery (Figure 2A). While the Buck et al. definition is not regulatory, it has been adopted by the California Biomonitoring Program (OEHHA, 2021).

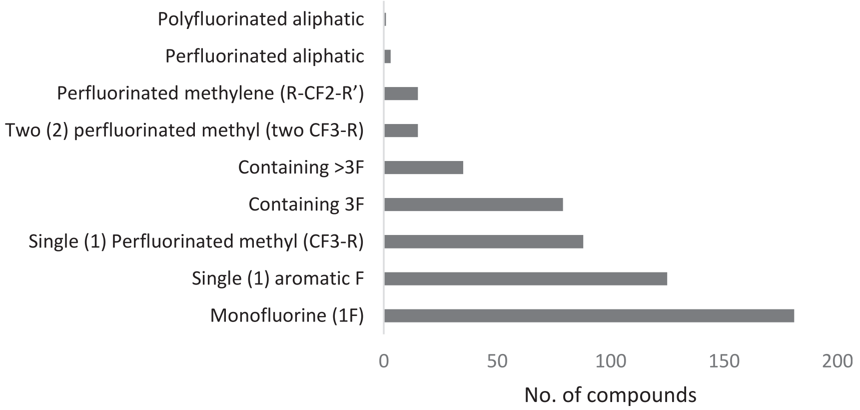


Figure 1. Substructures identified among organofluorine pharmaceuticals

PFAS identified by the Organisation for Economic Co-operation and Development (OECD)

The OECDoriginally defined PFAS as structures "that contain a perfluoroalkyl moiety with three or more carbons (i.e. $–C_nF_{2n}–$, $n \geq 3$) or a perfluoroalkylether moiety with two or more carbons (i.e. $–C_nF_{2n}OC_mF_{2m}–$, n and $m \geq 1$)" (OECD, 2018). Unlike Buck et al., this definition includes aromatic compounds. The OECD released a revised definition in 2021 including "fluorinated substances that contain at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it), i.e. with a few noted exceptions, any chemical with at least a perfluorinated methyl group ($–CF_3$) or a perfluorinated methylene group ($–CF_2–$)" (OECD, 2021). The revised definition reduced the number of carbons that must contain fluorine, but is clearer about the other atoms to which those carbons can be bonded. The 2018 OECD definition includes 5 (1.4%) organofluorine pharmaceuticals; the revised 2021 OECD definition includes 107 (30%) organofluorine pharmaceuticals. An example of a substance captured by the 2018 OECD definition but not Buck et al. is enflurane (Figure 2B). Included in the 2021 OECD definition but not Buck et al. are the cancer drug alpelisib (Figure 2C) and the widely used antidepressant fluoxetine (Prozac) (Figure 2G): the perfluorinated methyl groups warrant inclusion under the 2021 OECD definition, but the aromatic ring excludes them from Buck et al.

PFAS identified by Glüge et al.

The definition of Glüge et al. (2020) is broader than Buck et al., but narrower than the revised OECD 2021 definition (see Table 2 for the precise definition). Glüge et al. include aromatic compounds, similar to the OECD definition, yet does not include compounds with a single $–CF_3$ or $–CF_2–$, providing contrast to Buck et al. The antidiabetic medication gemigliptin meets the Glüge et al. definition because it is an aromatic substance that contains two perfluoroalkyl moieties on the side chains (Figure 2D). The Glüge et al. definition includes 22 (6.1%) organofluorine pharmaceuticals.

PFAS identified by the TURA Program of Massachusetts

The TURA Program originally defined PFAS as a compound containing "a perfluoroalkyl moiety with three or more carbons (e.g., $–C_nF_{2n}–$, $n \geq 3$; or $CF_3–C_nF_{2n}–$, $n \geq 2$) or a perfluoroalkylether moiety with two or more carbons (e.g., $–C_nF_{2n}OC_mF_{2m}–$ or $–C_nF_{2n}OC_mF_m–$, n and $m \geq 1$)" (Administrative Council on Toxics Use Reduction, 2021a). The slightly revised definition (Table 2) clarifies that the "–" excludes bonding to hydrogen. The original definition was ambiguous about this point and could be interpreted to include enflurane (Figure 2B) while the revised definition would not. Both would include perflexane (Figure 2E). The TURA 2021a definition includes six (1.7%) organofluorine pharmaceuticals while the revised definition includes four (1.1%).

PFAS identified by the U.S. EPA Office of Pollution Prevention and Toxics (OPPT)

The U.S. EPA OPPT defines PFAS as "… a structure that contains the unit $R-CF_2-CF(R')(R'')$, where R, R′, and R″ do not equal "H" and the carbon-carbon bond is saturated" (USEPA, 2021b). It also indicates that branched structures, heteroatoms, and cyclic structures are included. This definition is unambiguous, recognizing five (1.4%) organofluorine pharmaceuticals as PFAS. There were no compounds included

Table 3. Number of pharmaceuticals included under different definitions of PFAS (% of 360)

Definition	Number (%) organofluorine pharmaceuticals
Buck et al. (2011)	8 (2.2)
OECD (2018)	5 (1.4)
OECD (2021)	107 (30)
Glüge et al. (2020)	22 (6.1)
TURA (2021a)	6 (1.7)
TURA (2021b)	4 (1.1)
U.S. EPA OPPT (2021)	5 (1.4)
≥1 Fully Fluorinated Carbon[a]	337 (94)
All Organofluorine[b]	360 (100)

[a] Authorities whose legislation defines PFAS as a class of fluorinated organic chemicals containing at least one fully fluorinated carbon atom (NDAA, WA, ME, VT, CA).

[b] NGOs that advocate for broader definitions of PFAS to include all organofluorines.

under the OPPT definition that were not also captured by the 2021 OECDdefinition. Perflutren (Optison) is a contrast agent used in MRI and positron emission tomography (PET) imaging technology (Figure 2F). Perflutren meets all nine PFAS definitions examined as it is an aliphatic structure with three fully fluorinated carbon atoms (two perfluorinated methyl moieties and a perfluorinated methylene moiety).

PFAS identified by authorities as including at least one fully fluorinated carbon

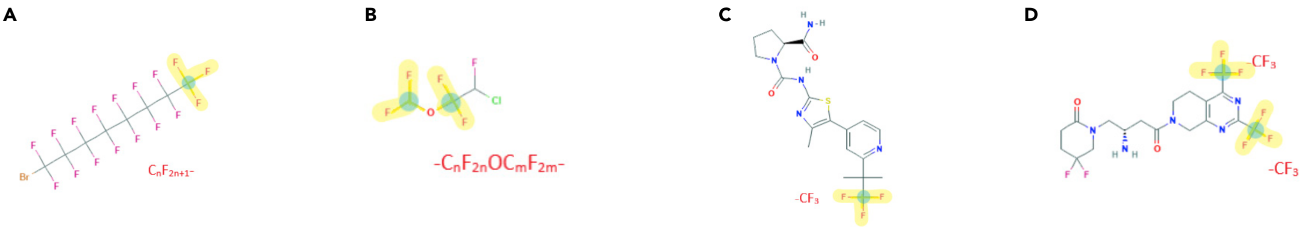
The U.S. NDAA defines PFAS as any substance containing "at least one fully fluorinated carbon" as do certain laws of the states of Washington, Vermont, Maine, and California (specific applications are discussed below). The NDAA defines a fully fluorinated carbon as "a carbon atom on which all of the hydrogen substituents have been replaced by fluorine" (116th Congress, 2019). However, the definition does not specify whether the fully fluorinated carbon is saturated or unsaturated (saturated compounds only contain single bonds). We therefore interpreted it to mean that the carbon could have single, double, or even triple bonds. This interpretation includes compounds containing a single fluorine atom attached to a benzene ring. As written, this definition captures 337 (94%) organofluorine pharmaceuticals. It includes the cholesterol-lowering medication atorvastatin (Lipitor), the top prescribed drug in the U.S. (Figure 2H) with 112,104,359 annual prescriptions (Table 4), as well as ciprofloxacin, a critical antibiotic (See Data S1). The ambiguity of the term "fully fluorinated carbon" is worth further consideration. If it had instead been interpreted to mean a trifluoromethyl group (R-CF_3) where R is not hydrogen, similar to Buck et al. (but without the latter definition's restriction to aliphatic compounds), neither Lipitor nor ciprofloxacin would be included, but Prozac (Figure 2G) would.

PFAS identified by non-governmental organizations: "all-organofluorine"

Some NGOs (Table 1) advocate for a broader definition of PFAS as any substance containing organofluorine. This definition is unambiguous and includes all 360 (100%) organofluorine pharmaceuticals, including widely used cancer chemotherapy drugs as well as Prozac and Lipitor discussed earlier.

DISCUSSION

The large number of PFAS listed by U.S. EPA and OECD suggests that research and regulation on a compound-by-compound basis is not practical. Multiple groups have devised definitions of PFAS to facilitate research into the prevalence, usage, and health effects of these substances, as well as serve as the basis for regulatory actions. Our analysis shows that the definitions have a very large range in the percent of organofluorine pharmaceuticals included. For this group of compounds, the definitions offer different and often conflicting views of what is and is not "PFAS". The framework we used is consistent with the systematic approach described in the OECD report (OECD, 2021) that provides practical guidance on characterizing PFAS based on molecular structure, and is similarly in line with the strategies described by (Wang et al., 2021) to facilitate unambiguous communication around PFAS. The cited examples serve to illustrate why PFAS definitions must be clear and that seemingly straightforward language—e.g., "fully fluorinated carbon"— can have multiple interpretations. Without specifying saturation (i.e., saturated compounds contain only single bonds), the fully fluorinated carbon definition can be interpreted to include any compound with

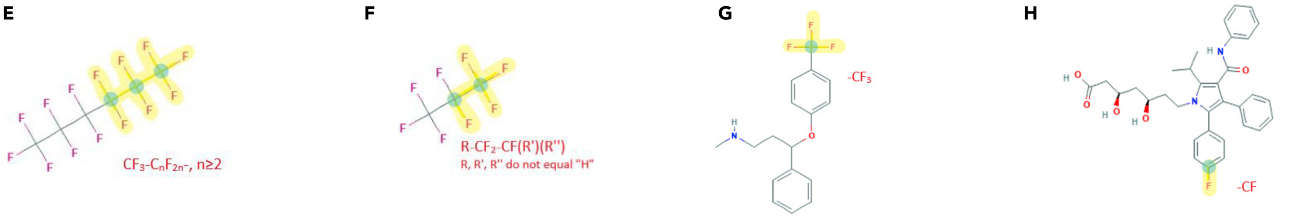


Perflubron
CAS No. 423-55-2

Enflurane
CAS No. 13838-16-9

Alpelisib
CAS No. 1217486-61-7

Gemigliptin
CAS No. 911637-19-9



Perflexane
CAS No. 355-42-0

Perflutren
CAS No. 76-19-7

Fluoxetine (Prozac)
CAS No. 54910-89-3

Atorvastatin (Lipitor)
CAS No. 134523-00-5

Figure 2. Examples of organofluorine pharmaceuticals that meet the nine PFAS definitions

(A) Buck et al. includes the contrast agent, perflubron (CAS No. 423-55-2).

(B) 2018 OECD and TURA 2021a both include the general anesthetic enflurane (CAS No. 13838-16-9).

(C) The 2021 OECD definition includes the antineoplastic alpelisib (CAS No.: 1217486-61-7).

(D) Glüge et al. includes the antidiabetic medication gemigliptin (CAS No. 911637-19-9).

(E) The TURA 2021b definition includes the cardiac ultrasound imaging agent perflexane (CAS No. 355-42-0).

(F) U.S. EPA OPPT includes the ultrasound contrast agent Perflutren (CAS No. 76-19-7).

(G) The ≥1 fully fluorinated carbon definition includes the antidepressant fluoxetine (Prozac) (CAS No. 54910-89-3).

(H) The "all-organofluorine" and ≥1 fully fluorinated carbon definitions include the cholesterol lowering medication atorvastatin (Lipitor) (CAS No. 134523-00-5).

a single aromatic fluorine, as well as other cases. While the definition was presumably intended to be clear and easy to interpret by stakeholders, it illustrates the importance of using specific and non-ambiguous language and being explicit in describing the context for which a definition shall be used.

To avoid confusion, it would ideally be useful to have a clear, universally agreed upon definition of PFAS. However, the appropriateness of a PFAS definition, or the possible need for exceptions in certain applications, may depend on the mandate of the group using the definition and its purpose. Of the nine definitions we have reviewed, five—Buck et al., OECD 2018 and 2021, Glüge et al., and "all organofluorines"—are non-regulatory at this time. The OECD, while not a regulatory institution, developed its own PFAS definition which may have regulatory implications if it is adopted by regulatory organizations, like the Registration, Evaluation, and Authorization of Chemicals (REACH) in the EU (European Commission, 2020). Five European countries (Germany, Netherlands, Denmark, Norway, and Sweden) announced their intention to develop a REACH restriction proposal for the European Commission that would cover all non-essential uses of PFAS in the EU (European Commission, 2020). Though not yet established at the time of this writing, this definition, if similar to the OECD, 2021 definition, may present important regulatory implications for the pharmaceutical industry and other producers of organofluorine chemicals.

Biomonitoring and environmental monitoring (e.g., of air and water) are critical surveillance aspects of environmental health. For example, biomonitoring of environmental chemicals is important for examining time trends (effectiveness of interventions, emerging problems, etc.) as well as geographical and demographic disparities and more. The definition used for PFAS has a potentially important role for biomonitoring, providing problem scoping, although there are practical limitations such as sample sizes, cost, availability of standards,

Table 4. Classification of organofluorine pharmaceuticals that rank in the top 500 U.S. prescribed drugs from 2019 and global sales in USD

Drug name	Brand name	Therapeutic class	Total R_X (2019)[a]	Drug rank[b]	Global sales 2018 (millions)[c]	All-organofluorine	≥1 Fully fluorinated carbon	OECD (2021)	TURA (2021a)	TURA (2021b)	Gluge et al	Buck et al	OECD (2018)	U.S. EPA OPPT
Flecainide	Tambocor	Tachyarrhythmia	2,318,516	215	296	X	X	X	X	X	X			
Fluoxetine	Prozac, Sarafem	antidepressant	27,110,302	20	945	X	X	X						
Celecoxib	Celebrex	NSAID; arthritis	6,595,235	102	3,980	X	X	X						
Levofloxacin	Iquix, Levaquin	Antibiotic	3,202,649	182	432	X	X	X						
Dexlansoprazole	Dexilant	proton pump inhibitor	2,290,526	218	3,831	X	X	X						
Leflunomide	Arava	rheumatoid arthritis	1,057,644	324	420	X	X	X						
Sulindac	Clinoril	NSAID	318,884	408	30	X	X	X						
Atorvastatin	Lipitor	cholesterol lowering agent	112,104,359	1	7,414	X	X							
Pantoprazole	Protonix	proton pump inhibitor	28,880,217	16	569	X	X							
Fluticasone propionate	Flonase	glucocorticoid (OTC)	27,893,102	18	791	X	X							
Escitalopram	Lexapro	antidepressant	27,510,958	19	1,282	X	X							
Rosuvastatin	Crestor	cholesterol lowering agent	27,041,319	21	n/a	X	X							
Citalopram	Celexa	antidepressant	21,546,700	30	n/a	X	X							
Sitagliptin	Januvia	antidiabetic	8,866,811	88	24,250	X	X							
Triamcinolone	Aristocort; Trianex	corticosteroid	6,320,751	107	n/a	X	X							
Ezetimibe	Zetia	cholesterol lowering agent	6,221,674	108	8,865	X	X							
Ciprofloxacin	Cipro	Antibiotic	5,878,441	113	488	X	X							
Fluconazole	Diflucan	antifungal	5,149,547	133	371	X	X							
Risperidone	Perseris Kit, Risperdal	antipsychotic	4,285,907	149	2,795	X	X							
Clobetasol	Clobex	corticosteroid	3,226,423	180	1,485	X	X							
Nebivolol	Bystolic	antihypertensive agent	3,061,887	191	2,800	X	X							
Ticagrelor	Brilinta	anticoagulant	2,299,436	216	3,007	X	X							
Ofloxacin	Floxin	antibiotic	2,051,823	232	153	X	X							

(*Continued on next page*)

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Table 4. *Continued*

Drug name	Brand name	Therapeutic class	Total R$_X$ (2019)[a]	Drug rank[b]	Global sales 2018 (millions)[c]	All-organofluorine	≥1 Fully fluorinated carbon	OECD (2021)	TURA (2021a)	TURA (2021b)	Gluge et al	Buck et al	OECD (2018)	U.S. EPA OPPT
Canagliflozin	Invokana	antidiabetic	1,373,540	290	4,327	X	X							
Betamethasone	Celestone, Alphatrex	corticosteroid	1,311,106	296	n/a	X	X							
Betamethasone dipropionate		corticosteroid	1,311,106	296	498	X	X							
Fluocinonide	Lidex	corticosteroid	1,290,749	300	555	X	X							
Travoprost	Izba, Travatan	glaucoma	1,264,924	303	2,722	X	X							
Difluprednate	Durezol	corticosteroid	717,461	356	587	X	X							
Dexamethasone	Decaderm, Decadron	corticosteroid	711,271	359	381	X	X							
Moxifloxacin	Avelox	antibiotic	666,288	363	n/a	X	X							
Fluorouracil	Adrucil, Carac, Efudex	antineoplastic	642,441	364	447	X	X							
Fluorometholone	Oxylone, Flarex	corticosteroid	434,531	389	161	X	X							
Fluocinolone acetonide	Flucinolone, Capex	corticosteroid	313,715	410	153	X	X							
Flurbiprofen	Ansaid	NSAID	21,338	477	6	X	X							
Emtricitabine	Emtriva	antiretroviral	3,632	501	5,457	X	X							
Paroxetine	Paxil	antidepressant	9,783,755	78	741	X								
Lansoprazole	Prevacid	propton pump inhibitor	2,772,218	200	963	X								
Diflunisal	Dolobid	NSAID	116,622	441	20	X								

[a] Annual prescription data for organofluorine pharmaceuticals are available from ClinCalc DrugStats database for the top 500 prescribed drugs in the U.S. for 2019.
[b] Drug Rank represents the rank order by frequency prescribed within a calendar year in the U.S.; data were compiled from the ClinCalc DrugStats database.
[c] Global sales data reported by PharmaCompass include prescriptions covered under Medicaid.

detection limits, etc. Biomonitoring programs may not be interested in organofluorine pharmaceuticals (e.g., the widely used Lipitor) themselves, except perhaps to try to close some of the gap between currently measured PFAS in serum vs. extractable organic fluorine (Yeung et al., 2008). Instead, biomonitoring programs would be more likely to examine the trends of known PFAS and add emerging compounds as they are discovered. California Biomonitoring currently uses the Buck et al. definition of PFAS (which would include very few organofluorine pharmaceuticals) (OEHHA, 2021). As discussed earlier, the PFAS definition included in the NDAA—which requires biomonitoring for PFAS among all military firefighters during their annual exam—uses the very broad and ambiguous "fully fluorinated carbon" definition, which includes over 90% of organofluorine drugs. Both of these applications may consider exempting such compounds.

On the other hand, monitoring of surface water, wastewater, biosolids, and other environmental media may be more interested in organofluorine pharmaceuticals as well as more traditional PFAS. Here, the definition of PFAS could well have regulatory implications and the choice of definition and possible exceptions would need to be carefully considered. For example, the NDAA applies the "fully fluorinated carbon" definition to environmental monitoring of PFAS in surface and groundwater by the United States Geological Survey (116th Congress, 2019). Recent efforts to measure total organic fluorine (TOF) in surface water (Ruyle et al., 2021) and in animal serum (Yeung et al., 2009) show that only a fraction of extractable organic fluorine (EOF) can be explained by known (targeted) PFAS, leaving a substantial portion of unidentified fluorine from other sources. Given the fate of organofluorine pharmaceuticals in wastewater, it is likely that these compounds would contribute to EOF measured in wastewater, and authorities that use the "fully fluorinated carbon" definition to measure or regulate PFAS will need to consider the implications for organofluorine pharmaceuticals. Alternatively, if the U.S. EPA OPPT definition were used, only a handful of organofluorine pharmaceuticals would be included. As a result, most pharmaceutical compounds, for which very little is understood on the biodegradability and recombination of breakdown products, would not be measured.

Four of the definitions we have considered—TURA 2021a/b, U.S. EPA OPPT, and the "fully fluorinated carbon" definition used by several states and the NDAA—have regulatory implications. There are important challenges around clarity and feasibility of regulating substances as a class. Ambiguities in how a definition is interpreted and applied can lead to misinterpretations by stakeholders, raising the likelihood of legal ramifications and ultimately slowing the process, potentially defeating the original goal of accelerating regulation through assessing PFAS on the basis of classes rather than individual chemicals. Earlier, we discussed the ambiguity in the "fully fluorinated carbon" definition and how it dramatically increased the number of organofluorine pharmaceuticals included. This would likely be true of other groups of organofluorine compounds not classified as PFAS under many of the other definitions.

Legislation in Washington, Vermont, California, and Maine (as well as the NDAA discussed above) each define PFAS as any compound containing at least one fully fluorinated carbon, but the applications differ. In California, the fully fluorinated carbon definition applies specifically to PFAS used in firefighting equipment and aqueous film forming foam (AFFF) (California, 2020). In Washington, this definition is applied to AFFF and food contact materials (Washington, 2021). Vermont applies the definition to AFFF as well as products added to rugs, food packaging, and ski wax (Vermont, 2021). When applied in these cases, the definition would not include organofluorine pharmaceuticals. Maine applies the fully fluorinated carbon definition in its legislation banning the selling or importing of any product containing intentionally added PFAS (Maine, 2021). The language of this legislation recognizes product categories in which the use of PFAS is currently unavoidable, which may include pharmaceuticals. Maine would also exempt pharmaceuticals because they are already regulated under federal law. Without this recognition, this law would include 94% of organofluorine pharmaceuticals.

The Massachusetts Toxic Use Reduction legislation provides an interesting example of exceptions. Certain industrial sectors are exempt from reporting toxic substances (MassDEP, 2018), including hospitals that may generate waste containing fluorinated contrast agents or other organofluorine pharmaceuticals used during hospital-based activities (e.g., surgical procedures, ventilation, etc.). Another approach to exceptions relevant to organofluorine pharmaceuticals is whether such products are deemed essential (Cousins et al., 2019).

Importantly, the list of organofluorine pharmaceuticals is dynamic and new drugs containing fluorine are developed each year. In fact, five organofluorine pharmaceuticals were approved during the final months of 2021, including Pfizer's new drug Paxlovid, the first protease inhibitor for treatment of SARS-CoV-2

(Pfizer, 2021). Pfizer signed a licensing agreement in November 2021 that will enable qualified manufacturers to produce and distribute the drug globally in order to reach a wider range of the global population (Pfizer, 2021). Paxlovid is an organofluorine pharmaceutical that meets the criteria of the revised OECD definition, the all-organofluorine definition, as well as the fully fluorinated carbon definition.

Moving forward with a useful framework

The definitions may be characterized by three attributes: clarity, inclusion, and specificity. Clarity may be interpreted as the degree to which a particular definition is open to conflicting decisions on whether a given PFAS structure meets the stated definition. Next, inclusion may be interpreted as the extent to which a definition would label any organofluorine compound as "PFAS", which we have illustrated here with pharmaceuticals. By specificity, we mean usefulness for its intended purpose. Specificity may be of particular importance to monitoring and regulatory bodies, which may need to consider exemptions for certain types of organofluorines if broad PFAS definitions are used. While consideration of these factors is important as we move forward, the real danger is not adopting any definition, for fear of not having a perfect definition, and the consequential delay in decision making.

Limitations of the study

This analysis considers nine available definitions of PFAS, yet new definitions may be developed for unique purposes, and previously established definitions may be revised in the future. Only those definitions available in the public space were included in this analysis. We include a comprehensive list of organofluorine pharmaceuticals approved between 1954 through June 1, 2021, including compounds that have been withdrawn. New therapeutics containing organofluorine approved after June 1, 2021 are not included. Our analysis is limited to human pharmaceuticals and does not include pharmaceuticals used in animals. Finally, available data on annual prescriptions are limited to the most widely prescribed drugs.

GLOSSARY

Aliphatic: saturated organic compounds in which the carbon atoms may form an open chain or closed rings

Alkyl group: a portion of a compound made up by carbon and hydrogen atoms arranged in a chain and whose structure follows the formula C_nH_{2n+1}

Aromatic: organic compounds containing a planar unsaturated ring of atoms that is stabilized by an interaction of the bonds forming the ring. Such compounds are typified by benzene and its derivatives

Ether: organic functional group typified by an oxygen atom connected to two carbon atoms, which may be aliphatic, olefinic, or aromatic.

Methyl group: a small molecule consisting of one carbon and three hydrogen atoms –CH3

Methylene group: a small molecule consisting of one carbon attached to two hydrogen atoms –CH2–

Moiety: a portion of a molecule with its own functional group

Olefinic: unsaturated organic compounds in which the carbon atoms may form an open chain or closed rings, including carbons that are double or triple bonded to another carbon.

Perfluorinated: a term to describe a hydrocarbon chain in which all of the hydrogen atoms are replaced by fluorine atoms

PFAS: per- and poly-fluoroalkyl substance

Polyfluorinated: a hydrocarbon chain in which multiple but not all hydrogen atoms are replaced by fluorine atoms

Polymer/polymeric: a class of compounds composed of macromolecules, usually consisting of multiple, repeating units called monomers

STAR★METHODS

Detailed methods are provided in the online version of this paper and include the following:

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  - Quantitative and qualitative analysis

SUPPLEMENTAL INFORMATION

Supplemental information can be found online at https://doi.org/10.1016/j.isci.2022.104020.

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AUTHOR CONTRIBUTIONS

Conceptualization, E.H., T.W., and W.H-B.; Methodology, E.H., T.W., R.G., and W.H-B.; Writing, E.H., T.W., W.H-B., and R.G.

DECLARATION OF INTERESTS

W.H-B and R.G. are members of the Toxic Use Reduction Institute Science Advisory Board in Massachusetts. The authors declare no other competing interests.

INCLUSION AND DIVERSITY

One or more of the authors of this paper self-identifies as a member of the LGBTQ+ community. One or more of the authors of this paper received support from a program designed to increase minority representation in science.

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STAR★METHODS

KEY RESOURCES TABLE

REAGENT or RESOURCE	SOURCE	IDENTIFIER
Other		
Chemical Structures and identifiers	National Library of Medicine PubChem Database	https://pubchem.ncbi.nlm.nih.gov/
Drug Database	KEGG Drug Databaste: Krypto Encyclopedia of Genes and Genomes	https://www.genome.jp/kegg/drug/
Prescription Drug Data	ClinCalc DrugStats Database	https://clincalc.com/
Global Sales Data	PharmaCompass Database	https://www.pharmacompass.com/

RESOURCE AVAILABILITY

Lead contact

Further information and requests for resources should be directed to and will be fulfilled by the lead contact, Emily Hammel (eghammel@bu.edu).

Materials availability

This study did not generate new materials.

Data and code availability

This paper analyzes existing, publicly available data. The data generated in this manuscript are supplied in a supplemental table. Any additional information required to reanalyze the data reported in this paper is available from the lead contact upon request. This paper does not report original code.

METHOD DETAILS

Identifying PFAS definitions

We selected and reviewed nine adopted definitions of PFAS that were available at the time of writing developed by both regulatory and non-regulatory organizations, presented in Table 1. Selection was based on the availability of a PFAS definition and a traceable description of the purpose for the development of the definition as it fits into the organizations' mandates or working scope. We present the organizations chronologically based on when the definition of PFAS was developed. For the purposes of direct comparison, we present the updated definitions for two of the organizations together with the originally developed definition.

Organofluorine pharmaceutical database

To establish a comprehensive list of organofluorine pharmaceuticals registered globally to date, we extended the work by Inoue et al. (2020), which included pharmaceuticals approved between 1954 and 2019, by querying the KEGG Drug database (Release version 99.1) for new organofluorine drugs approved between January 1, 2020 and June 1, 2021 (KEGG, 2021). KEGG Drug Database is a publicly available repository of approved drugs in the U.S., Europe and Japan, their chemical properties, and molecular structure, and other identifiers for prescription and over-the-counter (OTC) pharmaceuticals, including organofluorine pharmaceuticals that have been withdrawn either due to lack of demand or risk to patients.

The organofluorine pharmaceuticals identified from the KEGG Drug Database were queried using PubChem for the drug names, available synonyms, CAS registry number, molecular structure, chemical formula, InChI key, and therapeutic use area (Kim et al., 2019). Drug name refers to the generic pharmaceutical name; available brand names the pharmaceutical is sold under are listed separately as synonyms. Where available, the most recently collected data from 2019 on the number of U.S. prescriptions and the rank order by frequency prescribed within a calendar year were compiled from the ClinCalc DrugStats database (ClinCalc DrugStats Database, 2019) and are presented in Table 4 in addition to being made available in an Excel worksheet (Data S1). Drug utilization data from ClinCalc DrugStats was generated via the Agency for Healthcare Research and Quality's most recent Medical Expenditure Panel Survey (MEPS) from 2019, accessed in January 2022 (Agency for Healthcare Research and Quality, 2019). MEPS is a large-scale nationally representative survey of households and medical care providers across the U.S. and includes information on household-reported prescription drug use.

We also compile data on global sales and revenues from PharmaCompass, where available, on the organofluorine pharmaceuticals that rank in the top 500 prescribed drugs (PharmaCompass, 2021). ''Blockbuster'' drugs are defined as those whose global sales exceed $1B annually. Revenues can change from year to year based on whether a drug's patent is expired, and the availability of generics. It is more useful and consistent with the available data to compare the total number of prescriptions in a calendar year as a measure of how widely a drug is used. The pharmaceutical name and CAS registry number refers to the non-ionic form of the drug, unless the ionic equivalent is necessary for identification in which case both forms are included. Ionic equivalents are presented primarily for corticosteroids in which case multiple ionic forms of the compounds have distinct clinical uses. For example, fluoxetine hydrochloride is presented simply as fluoxetine whereas fluticasone propionate and fluticasone furoate are presented separately since they are different drugs with unique pharmacological activity.

Quantitative and qualitative analysis

Each of the identified organofluorine pharmaceutical structures were reviewed against the nine definitions. The definitions were ranked from most to least inclusive with the most inclusive definition containing the largest number of compounds. We describe ambiguities in some definitions with examples.

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Article

Unknown Organofluorine Mixtures in U.S. Adult Serum:Contribution from Pharmaceuticals?

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Abstract: Organofluorines occur in human serum as complex mixtures of known and unidentified compounds. Human biomonitoring traditionally uses targeted analysis to measure the presence of known and quantifiable per- and polyfluoroalkyl substances (PFAS) in serum, yet characterization of exposure to and quantification of PFAS are limited by the availability of methods and analytical standards. Studies comparing extractable organofluorine (EOF) in serum to measured PFAS using organofluorine mass balance show that measurable PFAS only explain a fraction of EOF in human serum and that other sources of organofluorine may exist. The gap in fluorine mass balance has important implications for human biomonitoring because the total body burden of PFAS cannot be characterized and the chemical species that make up unidentified EOF are unknown. Many highly prescribed pharmaceuticals contain organofluorine (e.g., Lipitor, Prozac) and are prescribed with dosing regimens designed to maintain a therapeutic range of concentrations in serum. Therefore, we hypothesize organofluorine pharmaceuticals contribute to EOF in serum. We use combustion ion chromatography to measure EOF in commercial serum from U.S. blood donors. Using fluorine mass balance, we assess differences in unexplained organofluorine (UOF) associated with pharmaceutical use and compare them with concentrations of organofluorine predicted based on the pharmacokinetic properties of each drug. Pharmacokinetic estimates of organofluorine attributable to pharmaceuticals ranged from 0.1 to 55.6 ng F/mL. Analysis of 44 target PFAS and EOF in samples of commercial serum (n = 20) shows the fraction of EOF not explained by Σ_{44} PFAS ranged from 15% to 86%. Self-reported use of organofluorine pharmaceuticals is associated with a 0.36 ng F/mL (95% CL: −1.26 to 1.97) increase in UOF, on average, compared to those who report not taking organofluorine pharmaceuticals. Our study is the first to assess sources of UOF in U.S. serum and examine whether organofluorine pharmaceuticals contribute to EOF. Discrepancies between pharmacokinetic estimates and EOF may be partly explained by differences in analytical measurements. Future analyses using EOF should consider multiple extraction methods to include cations and zwitterions. Whether organofluorine pharmaceuticals are classified as PFAS depends on the definition of PFAS.

Keywords: per- and polyfluoroalkyl substances; human biomonitoring; targeted analysis; extractable organofluorine; pharmaceuticals

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1. Introduction

Per- and polyfluoroalkyl substances (PFAS) are a class of thousands of anthropogenic chemicals widely used in commercial products, industrial manufacturing, food packaging, pesticides, and aqueous film-forming foams for their durable and water-repellant properties [1]. PFAS are widely detected in the environment, in wildlife, and in humans [2–7]. A number of adverse health effects are associated with low levels of some PFAS in serum [8–13]. Traditional human biomonitoring studies measure 6–12 PFAS in serum [14], yet upwards of 12,000 individual PFAS are reported to exist [15]. The large number of PFAS makes a chemical-by-chemical approach to investigation unworkable, and class-based

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approaches to identify and track PFAS in humans and the environment based on their chemical structure have been proposed [16–20]. Further challenges are the differences in the definition of a PFAS [21]. Characterizing exposure to the full suite of PFAS is also limited by current analytical methods, which can only quantify exposure to compounds for which analytical standards exist and are readily available. Most of what is known about the health risks associated with PFAS comes from data on a very small subset of PFAS [22], yet less is known about the thousands of other PFAS in commerce [3].

Observations from the 1960s showed inorganic fluoride only partly explained the mass of total fluorine in serum, revealing unknown sources of organofluorine in serum [23]. In the 1990s and early 2000s, the identities of PFOA, PFOS, and other PFAS with industrial uses in the latter half of the 20th century were established [24], yet there remains a gap in our knowledge of the contributors to the fluorine detected in serum. Novel methods using combustion ion chromatography (CIC) for fluorine show large amounts of extractable organofluorine (EOF) in serum [25]. Using fluorine mass balance approaches, pioneering studies have shown that *conventional* PFAS—defined here as those with industrial uses and their precursors and replacements that are typically measured in human biomonitoring—only partly explain EOF in serum, with the fraction of unexplained organofluorine (UOF) ranging from 24% to 89% [25–28].

There are a number of potential types of UOF in human serum. (1) Replacements for conventional PFAS or their precursors, for which analytical standards are not available. For example, perfluoroalkyl acid (PFAA) precursors can be metabolized in humans to form terminal PFAS species [2], but the vast array of PFAS precursors as well as their respective intermediates are not quantifiable using traditional liquid chromatography mass spectrometry (LC-MS/MS) techniques [27,29–31]. (2) Ultra-short-chain PFAS that are not typically biomonitored. For example, trifluoroacetic acid (TFA) is a breakdown product of some organofluorine compounds that is frequently detected in the environment but only rarely measured in serum [27]. (3) Organofluorine pharmaceuticals. (4) Other organofluorine compounds, including pesticides. Whether these additional sources contribute to UOF as "PFAS" depends on the structural definition of PFAS being used.

Many highly prescribed pharmaceuticals contain organofluorine and can be classified as PFAS under some definitions [21]. Organofluorine has been used in the pharmaceutical industry since 1954 and is useful in altering the physiochemical properties of a drug to achieve a desired pharmacological effect [32]. Today, roughly 20% of pharmaceuticals currently registered with the FDA contain organofluorine [32], including the frequently prescribed anti-depressant Prozac, the protease inhibitor Paxlovid used for treating COVID-19, and Lipitor, the top-prescribed medication in the U.S. and used to lower cholesterol. With the correct dosing regimen, pharmaceuticals are prescribed in such a way that they remain present in serum within a clinically effective range [33].

We hypothesize that a portion of UOF in serum is attributable to organofluorine pharmaceuticals. In this pilot study using human serum, we used fluorine mass balance to assess differences in UOF associated with reported pharmaceutical use and compared them with concentrations of organofluorine predicted based on the pharmacokinetic properties of each pharmaceutical. To our knowledge, this is the first study to use CIC for fluorine to measure EOF in U.S. serum and determine the fraction of EOF not explained by conventional PFAS.

2. Materials and Methods

2.1. Organofluorine Pharmaceutical Selection

To identify highly prescribed organofluorine pharmaceuticals likely to be used among a random sample of U.S. adults, we used the list of 340 organofluorine pharmaceuticals approved in the U.S., Japan, and Europe between 1954 and 2019 generated by Inoue et al. [32] based on the publicly available KEGG drug database [34]. The KEGG Drug Database is a publicly available repository of approved drugs in the U.S., Europe, and Japan, which includes their chemical properties and molecular structures, as well as other identifiers for prescription and over-the-counter (OTC) pharmaceuticals. Cross-referencing the 340 organofluorine pharmaceuticals with drug utilization data from the ClinCalc Drug Database (version 2022.08) [35], we identified nine organofluorine pharmaceuticals that ranked among the top 100 prescribed drugs in the U.S. in 2020 (Table 1), therefore representing the organofluorine pharmaceuticals most likely to be used among U.S. adults.

Table 1. Top nine U.S. prescribed organofluorine pharmaceuticals, names, uses, chemical properties, and pharmacokinetic-based estimates of organofluorine in order of U.S. prescriptions (2020).

Pharmaceutical Information				**Chemical Properties**						
Generic Name	**Brand Name**	**Therapeutic Use**	**U.S. Prescriptions (2020)**	**Molecular Formula**	**Molecular Weight (g/mol)**	**Dissociation Constant (pka) [a]**	**#F**	**Fraction F**	**Estimated Serum Levels (ng/mL) [b]**	**Estimated Organofluorine (ng F/mL)**
Atorvastatin	Lipitor	statin	114,509,814	$C_{33}H_{35}FN_2O_5$	558.65	4.31	1	0.034	2.4–11.2 [d]	0.1–0.4
Escitalopram	Lexapro	SSRI	30,605,646	$C_{20}H_{21}FN_2O$	324.40	9.78	1	0.059	15–80 [e]	0.9–4.7
Rosuvastatin	Crestor	Statin	29,750,488	$C_{22}H_{28}FN_3O_6S$	481.54	4.00	1	0.039	1.8–7.4 [f, g]	0.1–0.3
Pantoprazole	Protonix	Proton-pump inhibitor	26,604,040	$C_{16}H_{15}F_2N_3O_4S$	383.37	3.92 (SB) 8.19 (SA)	2	0.099	39.9–87.9	4.0–8.7
Fluticasone [c]	Flonase	intranasal corticosteroid	24,777,490	$C_{22}H_{27}F_3O_4S$	444.51	−3.4 (SB) 13.56 (SA)	3	0.128	N/A	N/A
Fluoxetine	Prozac	SSRI	23,403,050	$C_{17}H_{18}F_3NO$	309.33	9.80	3	0.184	91–302	15.8–55.6
Citalopram	Celexa	SSRI	18,549,176	$C_{20}H_{21}FN_2O$	324.40	9.78	1	0.059	50–100 [e]	2.9–6.4
Sitagliptin	Januvia	anti-diabetic	9,885,657	$C_{16}H_{18}F_6N_5O_5P$	407.32	8.78	6	0.280	165	46.3
Paroxetine	Paxil	SSRI	9,029,667	$C_{19}H_{20}FNO_3$	329.37	9.77	1	0.058	30–120 [e]	1.7–6.9

Notes: [a] pKa values obtained from DrugBank Database [36].; [b] All pharmacokinetic data obtained from FDA drug labels unless otherwise noted.; [c] Limited pharmacokinetic information available for oral inhalation of Fluticasone.; [d] Lins et al., 2003 [37]; [e] Mayo Clinic Labs Test Catalog [38]; [f] Li et al., 2010 [39]; [g] Martin et al., 2002 [40]; Abbreviations: SSRI: selective serotonin reuptake inhibitor; Pantoprazole and Fluticasone are zwitterions with multiple functional groups; pKa values are provided for each functional group, denoted as strongest acid (SA) and strongest base (SB).

2.2. Pharmacokinetic Estimates

We used the pharmacokinetic properties of the nine organofluorine pharmaceuticals shown in Table 1 to estimate the concentration of organofluorine in serum attributable to each of these compounds. Pharmaceuticals are prescribed to maintain blood concentrations within a therapeutic range, i.e., the steady state. The average concentration at steady state is commonly used to estimate levels of a compound in serum. For purposes of this analysis, we assumed steady-state concentrations for each of the nine pharmaceuticals were achieved given that all the compounds are prescribed for chronic conditions [21] with dosing regimens that aim to maintain relatively constant levels of the compound within a therapeutic range. Pharmacokinetic information was obtained from FDA drug labels when available and from the clinical literature when FDA drug labels were incomplete. For each pharmaceutical, the estimated range of serum levels of the parent compound (ng/mL) was represented by the range of average plasma concentrations at steady state (C_{SS}). When available, we used the range of average plasma concentrations reported in the drug label or the literature. Otherwise, we used the pharmacokinetic parameters in Equation (1) to determine the average plasma concentration at steady state.

$$C_{SS} = \frac{AUC}{\tau} \tag{1}$$

C_{SS} is the average concentration at steady state (ng/mL), the area under the curve (AUC) is equivalent to the total exposure to the compound over the course of the dosing interval (ng*h/mL), and τ is the duration of the dosing interval in hours (h).

To determine the concentration of organofluorine in serum attributable to a given compound, we multiplied the proportion of the compound due to fluorine by the serum concentration of the compound (Equation (2)) [27].

$$\boldsymbol{C_F = \left(\#\, flourine\ atoms \times \frac{MW_F}{MW_C}\right) \times C} \tag{2}$$

where C_F (ng F/mL) is the concentration of the compound in equivalents of fluorine, MW_F is the atomic weight of fluorine (g/mol), MW_C is the molecular weight of the compound (g/mol), and C is the concentration of the compound in serum (ng/mL), for pharmaceuticals the range of steady-state concentrations.

2.3. Serum Procurement and Sampling Protocol

All serum samples were sourced commercially from BioIVT Laboratory Services (Westbury, NY, USA), a biospecimen procurement company. Samples were collected from consenting donors by BioIVT at blood collection centers across the U.S. between 10 December 2020, and 18 January 2021 [41]. Per this study-specified sampling protocol, donors ages 25–65 with no previous history of taking cholestyramine (Questran), a cholesterol-lowering medication associated with increased elimination of PFAS [42], were eligible for inclusion in the study. At the time of sample collection, donors were verbally screened by BiolVT to ascertain their current medication use, and information was collected on donor demographics related to age, sex, and race/ethnicity.

We provided BioIVT with a list of the generic drug names and corresponding brand names for the nine organofluorine pharmaceuticals in Table 1. Serum was collected from ten males and ten females, half of whom reported using one or more of the nine organofluorine pharmaceuticals at the time of sampling, and the other half reported not using these pharmaceuticals. We classified the first group as pharmaceutical users and the second as non-users.

2.4. Sample Handling

As per BioIVT internal standard operating procedures, individuals' whole blood was drawn into a 500 mL dry collection bag (Terumo BCT, INC., Lakewood, CO, USA, model 1BB*D606A) and spun at 5000× g for 10 min at −5 °C. The supernatant liquid was transferred into another bag and allowed to clot at room temperature for up to 48 h, and then spun at 5000× g for 20 min at −4 °C. The supernatant liquid was aliquoted into individual 3 mL vacutainers, frozen on dry ice for transport, and shipped via Boston University SPH to Örebro University, Örebro, Sweden, where it was stored at −20 °C and analyzed for PFAS and EOF.

2.5. Sample Extraction

The sample extraction method used was based on an ion-pair extraction method originally published by Hansen et al. [24] and later modified in this study. In brief, the samples were extracted in duplicate; the first subsample (Replicate 1) was used for target analysis (spiked with an internal standard), and the second subsample (Replicate 2) was used for EOF analysis (no internal standard added). First, 2 mL of a 0.5 M TBA solution in water was added to the sample and vortex mixed; then, 5 mL of MTBE was added to the mixture. The mixture was shaken horizontally at 250 rpm for 15 min and then centrifuged for 10 min at 8500 rpm (8000× g). The extraction was repeated twice with 3 mL of MTBE instead of 5 mL after collecting the organic solvent layer. The organic solvent extracts from all three cycles were combined and evaporated to 0.2 mL under a stream of nitrogen, then reconstituted to 1.0 mL with MeOH and evaporated to a final volume of 0.5 mL for instrumental analysis.

2.6. Instrumental Analysis and Quantification

The analysis and quantification have been described in detail previously [43]. In brief, the target analytes were quantified using an Acquity ultra-performance liquid chromatograph (UPLC) with a Xevo TQ-S micro tandem mass spectrometer (MS/MS). Both instruments were from the Waters Corporation (Milford, MA 01757, United States). The target analytes were separated using a C18 BEH column (2.1 × 100 mm, 1.7 μm); the mobile phases were a 30/70 (v/v) mixture of MeOH and water and 100% MeOH. Both mobile phases had 5 mmol/L 1-methylpiperidine and 2 mmol/L ammonium acetate as additives [44]. The 44 target PFAS included legacy compounds, potential precursors, and novel PFAS species, which were quantified using internal calibration with corresponding internal standards (mass-labelled standards). For those without a corresponding internal standard, the compound with the closest retention time of the same compound class was used. Details of the list of internal standards used can be found elsewhere [27]. Repeated injections of a standard mixture during analytical runs were used to monitor the performance of the UPLC-MS/MS system.

A combustion ion chromatography (CIC) system was used to determine EOF content. The CIC system was made of a combustion module (Analytik Jena, Germany), a 920 absorber module (Metrohm, Switzerland), and a 930 compact IC flex ion chromatograph module (Metrohm, Switzerland). EOF analysis results are described in ng F/g, which are equivalent to the concentration of fluorine in serum (ng F/mL) using the density of serum (~1 g/mL). Separation was achieved using an ion-exchange column (Metrosep A Supp 5–150/4.0), and the mobile phase was a carbonate buffer (64 mmol/L sodium carbonate and 20 mmol/L sodium bicarbonate). Water was used as the absorber solution. An external calibration curve, produced by combusting PFOA (Aldrich, Burlington, United States), was used for quantification.

The quality assurance and quality control (QA/QC) measures, including the performance of samples using SRM1957 and the relative standard deviation (RSD) of QC samples consisting of PFOS and PFOA, recoveries of target PFAS, as well as repeatability of the CIC system, are described in more detail elsewhere [43]. The limits of quantification (LOQ) of individual PFAS ranged from 0.020 to 0.065 ng/mL (Supplemental Information Table S1). To calculate ΣPFAS values, measurements of target PFAS below the LOQ were substituted with the value of zero, as described elsewhere [43]. The LOQ (3.8 ng F/g) of EOF using CIC was calculated as the average of three procedural blanks plus three times the standard deviation of the procedural blanks before applying any concentration factor for the volume of blood used. Samples with values below the LOQ were replaced with the LOQ value divided by the concentration factor of the sample. Reported sample concentrations might result in lower values than the LOQ value due to different concentration factors (SI Table S2).

2.7. Organofluorine Mass Balance

Individual PFAS concentrations were converted to fluorine-equivalent concentrations using Equation (2), where C is now the serum concentration of the PFAS determined using LC-MS/MS. The known EOF for the measured 44 PFAS ($\Sigma\ C_{\text{F-PFAS}}$; ng F/mL) was determined by summing the fluorine concentrations attributable to Σ_{44} PFAS. The concentration of unknown organofluorine (C_{UOF}; ng F/mL) was calculated as the difference between the concentration of total EOF (C_{EOF}; ng F/mL) and known EOF ($\Sigma\ C_{\text{F-PFAS}}$; ng F/mL).

2.8. Statistical Analysis

We used the Shapiro–Wilks test to assess the normality of the concentration of UOF. Since the distribution of UOF concentration was approximately normal, bivariate analyses were conducted using two sample t-tests to assess differences in UOF across sex, race/ethnicity, and age (treated as a dichotomous variable with observations falling above or below the median of 48.5 years). We used Spearman's rank correlation to determine whether the concentration of UOF is associated with the concentration of organofluorine attributable to target PFAS.

We used linear regression to determine the crude difference in the concentration of UOF between donors who reported use of organofluorine pharmaceuticals and those who did not. Based on the results of bivariate analyses, we used multiple linear regression to consider the effect of age as a potential confounder in our estimates of the effect of pharmaceutical use on UOF. We performed regression diagnostics to confirm the assumptions of homoscedasticity, linearity, and independence were met and to identify potential influence points and outliers.

Given the skewed distribution of PFAS measured in both groups, we used the Wilcoxon rank-sum test to compare the distributions of Σ_{44} PFAS between pharmaceutical users and donors who reported no pharmaceutical use. To compare our sample with national levels reported by the National Health and Nutrition Examination Survey (NHANES), we compared the median concentrations of a subset of Σ_5 PFAS monitored by NHANES for U.S. adults in 2017–2018 and detected in >95% of donated sera (n = 20): PFOA, PFOS, PFHxS, PFHpS, and PFNA (SI Table S2) [45].

3. Results

3.1. Pharmacokinetic Estimates of Serum Fluorine

Estimated serum organofluorine concentrations for each of the nine pharmaceuticals are presented in Table 1. Concentrations of organofluorine attributable to each pharmaceutical range from 0.1 to 55.6 ng F/mL, directly influenced by the number of fluorine atoms in their molecular structure. Atorvastatin (Lipitor), estimated to contribute 0.1–0.4 ng F/mL, is the most widely used drug of the nine, with over 114 million U.S. prescriptions per year in 2020. On the high end, Fluoxetine (Prozac) contributes 15.8–55.6 ng F/mL with 23 million prescriptions per year. Two compounds, Citalopram and Escitalopram, share the same molecular formula, but the former is a mixture of two enantiomers while the latter is one enantiomer and is prescribed at half the dose, explaining why the estimated levels of organofluorine in serum differ by a factor of two.

3.2. Characteristics of Study Serum Donors and PFAS Concentrations

Demographic data for the serum donor population are presented in Table 2, PFAS results are presented in Table 3, and Supplemental Information is presented in Table S2. Donors that reported using pharmaceuticals were on average five years older than donors with no reported pharmaceutical use but did not differ in their median age (Table 2). Pharmaceutical users had somewhat higher serum concentrations of Σ_{44} PFAS (Table 3).

Table 2. Demographic data for blood donors (n = 20). Donors who reported a history of taking Questran were excluded.

	No Reported Pharma Use (n = 10) n (%)	**Reported Pharma Use (n = 10) n (%)**
Sex		
Male	5(50)	5(50)
Female	5(50)	5(50)
Race		
Black	4(40)	4(40)
Hispanic	6(60)	6(60)
Age		
mean (±SD)	45 (±11.8)	50 (±13.4)
median	49	48.5
range	28–59	32–74