Making an imPACt

Source-based Nomenclature for Single-strand Homopolymers and Copolymers (IUPAC Recommendations 2016)

Richard G. Jones, et al.

Pure and Applied Chemistry, 2016

Volume 88, Issue 10-11, pp. 1073-1100

IUPAC recommendations on source-based nomenclature for single-strand polymers have so far addressed its application mainly to copolymers, non-linear polymers and polymer assemblies, and within generic source-based nomenclature of polymers. In this document, rules are formulated for devising a satisfactory source-based name for a polymer, whether homopolymer or copolymer, which are as clear and rigorous as possible. Thus, the source-based system for naming polymers is presented in a totality that serves as a user-friendly alternative to the structure-based system of polymer nomenclature. In addition, because of their widespread and established use, recommendations for the use of traditional names of polymers are also elaborated.

http://dx.doi.org/ 10.1515/pac-2015-0702

Comprehensive Definition of Oxidation State (IUPAC Recommendations 2016)

Pavel Karen, Patrick McArdle, and Josef Takats *Pure and Applied Chemistry*, 2016 Volume 88, Issue 8, pp. 831-839

Oxidation state (OS) gives the degree of oxidation of an atom in terms of counting electrons. [1] It scales trends in redox and acid-base properties, as well as in physical properties such as magnetism, and is a key component when tracking the course of chemical reactions. Thus, the concept of OS is important, and so is an agreed upon definition of what OS is and the algorithmic manner in which it is to be calculated. In the absence of an actual definition, algorithms have thus far been used to define OS.

This recommendation proposes a definition of OS based on ionic approximation of chemical bonds, illustrated on a molecular-orbital scheme and deduced from electronegativity considerations (Allen's scale). Two algorithms are formulated for the determination of OS in molecules, ions, and extended solids, and are illustrated with examples. Limits, beyond which OS ceases to be well-defined or becomes ambiguous, are

The full scholarly paper providing the 2014 self-consistent set of values of the constants and conversion factors of physics and chemistry recommended by the Committee on Data for Science and Technology (CODATA) was published in September 2016 in Review of Modern Physics 88, 035009 (2016); https://doi.org/10.1103/RevModPhys.88.035009. The full text article, a wall chart, and a wallet card (reprint below) are available from the NIST website at http://physics.nist.gov/cuu/Constants

2014 CODATA RECOMMENDED VALUES OF THE FUNDAMENTAL CONSTANTS OF PHYSICS AND CHEMISTRY NIST SP 959 (Aug 2015)

See: P. J. Mohr, D. B. Newell, and B. N. Taylor, arxiv.org/pdf/1507.07956v1.pdf (2015). A more extensive listing of constants is available in the reference given above and on the NIST Physical Measurement Laboratory Web site: physics.nist.gov/constants.

Quantity	Symbol	Numerical value	Unit
speed of light in vacuum	c, c_0	299 792 458 (exact)	$\mathrm{m}\;\mathrm{s}^{-1}$
magnetic constant	μ_0	$4\pi \times 10^{-7}$ (exact)	$N A^{-2}$
electric constant $1/\mu_0 c^2$	ϵ_0	$8.854187817\times10^{-12}$	$\mathrm{F}\ \mathrm{m}^{-1}$
Newtonian constant of gravitation	n G	$6.67408(31) \times 10^{-11}$	$m^3 kg^{-1} s^{-2}$
Planck constant	h	$6.626070040(81) \times 10^{-34}$	Jѕ
$h/2\pi$	\hbar	$1.054571800(13) \times 10^{-34}$	Jѕ
elementary charge	e	$1.6021766208(98)\times10^{-19}$	\mathbf{C}
fine-structure constant $e^2/4\pi\epsilon_0\hbar c$	α	$7.2973525664(17) \times 10^{-3}$	
inverse fine-structure constant	α^{-1}	137.035999139(31)	
Rydberg constant $\alpha^2 m_{\rm e} c/2h$	R_{∞}	10973731.568508(65)	m^{-1}
Bohr radius $\alpha/4\pi R_{\infty}$	a_0	$0.52917721067(12)\times10^{-10}$	m
Bohr magneton $e\hbar/2m_{\rm e}$	$\mu_{ m B}$	$927.4009994(57) \times 10^{-26}$	${ m J} { m T}^{-1}$

exemplified; moving outside these requires additional measurements, round offs, estimates, or plain postulates. Specific uses that justify a nominal OS are also explained.

http://dx.doi.org/10.1515/pac-2015-1204

Glossary of Terms Used in Developmental and Reproductive Toxicology (IUPAC Recommendations 2016)

John H. Duffus, Michael Schwenk, and Douglas M. Templeton *Pure and Applied Chemistry*, 2016 Volume 88, Issue 8, pp. 713-830

The primary objective of this glossary is to give clear definitions for those who contribute to studies relevant to developmental and reproductive toxicology, or who must interpret them, but are not themselves reproductive physiologists or physicians. This applies especially to chemists who need to understand the literature of reproductive and teratogenic effects of substances without recourse to a multiplicity of other glossaries or dictionaries. The glossary includes terms related to basic and clinical reproductive biology and teratogenesis, insofar as they are necessary for a self-contained document, particularly terms related to

diagnosing, measuring, and understanding the effects of substances on the embryo, on the fetus, and on the male and female reproductive systems. The glossary consists of about 1200 primary alphabetical entries and includes Annexes of common abbreviations and examples of chemicals with known effects on human reproduction and development. The authors hope that, in addition to chemists, toxicologists, pharmacologists, medical practitioners, risk assessors, and regulatory authorities are among the groups who will find this glossary helpful. In particular, the glossary should facilitate the worldwide use of chemical terminology in relation to occupational and environmental risk assessment.

http://dx.doi.org/10.1515/pac-2015-1202

Quantity	Symbol	Numerical value	Unit
electron mass	$m_{ m e}$	$9.10938356(11)\times10^{-31}$	kg
proton mass	$m_{ m p}$	$1.672621898(21) \times 10^{-27}$	kg
proton-electron mass ratio	$m_{ m p}/m_{ m e}$	1836.15267389(17)	
Avogadro constant	$N_{ m A}, L$	$6.022140857(74)\times10^{23}$	mol^{-1}
Faraday constant $N_{\rm A}e$	F	96 485.332 89(59)	$C \text{ mol}^{-1}$
molar gas constant	R	8.314 4598(48)	$\mathrm{J} \; \mathrm{mol^{-1}} \; \mathrm{K^{-1}}$
Boltzmann constant $R/N_{\rm A}$	k	$1.38064852(79) \times 10^{-23}$	$\rm J~K^{-1}$
Stefan-Boltzmann const. $\pi^2 k^4/60\hbar^3 c^2$	σ	$5.670367(13) \times 10^{-8}$	${ m W} { m m}^{-2} { m K}^{-4}$
magnetic flux quantum $h/2e$	Φ_0	$2.067833831(13)\times 10^{-15}$	Wb
Josephson constant $2e/h$	$K_{ m J}$	$483597.8525(30) \times 10^9$	$\mathrm{Hz}\ \mathrm{V}^{-1}$
von Klitzing constant h/e^2	$R_{ m K}$	25 812.807 4555(59)	Ω
electron volt (e/C) J	eV	$1.6021766208(98)\times10^{-19}$	J
(unified) atomic mass unit $\frac{1}{12}m(^{12}C)$	u	$1.660539040(20)\times10^{-27}$	kg

The number in parentheses is the one-sigma (1 σ) uncertainty in the last two digits of the given value.

