

Names for hydrogen atoms, ions, and groups, and for reactions involving them (recommendations 1988)

BUNNETT, J.F., JONES, R.A.Y. & IUPAC Commission on Physical Organic Chemistry

MULLER, Paul (Collab.)

Reference

BUNNETT, J.F., JONES, R.A.Y. & IUPAC Commission on Physical Organic Chemistry, MULLER, Paul (Collab.). Names for hydrogen atoms, ions, and groups, and for reactions involving them (recommendations 1988). *Pure and Applied Chemistry*, 1988, vol. 60, no. 7, p. 1115-1116

DOI : 10.1351/pac198860071115

Available at:

<http://archive-ouverte.unige.ch/unige:152888>

Disclaimer: layout of this document may differ from the published version.



UNIVERSITÉ
DE GENÈVE

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

ORGANIC CHEMISTRY DIVISION
COMMISSION ON PHYSICAL ORGANIC CHEMISTRY*

NAMES FOR HYDROGEN ATOMS, IONS, AND GROUPS, AND FOR REACTIONS INVOLVING THEM

(Recommendations 1988)

Prepared for publication by

J. F. BUNNETT¹ and R. A. Y. JONES²

¹University of California, Santa Cruz, USA

²University of East Anglia, Norwich, UK

*Membership of the Commission during the period (1983–1987) this report was prepared was as follows:

V. Gold† (UK, *Chairman*: 1983–85); P. Müller (Switzerland, *Chairman*: 1985–1987); R. A. Y. Jones (UK, *Secretary*: 1983–87); T. A. Albright (USA, National Representative); P. Ahlberg (Sweden, National Representative); A. T. Balaban (Romania, National Representative); J. F. Bunnett (USA, Associate); M. P. Doyle (USA, Associate); W. Drenth (Netherlands, National Representative); R. D. Guthrie (USA, Associate); E. A. Halevi (Israel, Titular); J. J. E. Humeres A. (Brazil, National Representative); G. Illuminati† (Italy, Titular); W. P. Jencks (USA, Titular); Jiang Xikui (China, National Representative); P. Laszlo (Belgium, National Representative); J. S. Littler (UK, Associate); D. J. McLennan (New Zealand, National Representative); J. March (USA, Associate); M. Mihailovic (Yugoslavia, National Representative); O. Nefedov (USSR, Titular); M. Nogradi (Hungary, National Representative); M. Oki (Japan, Titular); J. Penton (Switzerland, Associate); K. Schwetlick (GDR, Titular); J. Toullec (France, Associate); P. van Brandt (Belgium, Associate); Z. Zavada (Czechoslovakia, National Representative); J. Zdysiewicz (Australia, National Representative).

† deceased

Republication of this report is permitted without the need for formal IUPAC permission on condition that an acknowledgement, with full reference together with IUPAC copyright symbol (© 1988 IUPAC), is printed. Publication of a translation into another language is subject to the additional condition of prior approval from the relevant IUPAC National Adhering Organization.

Names for hydrogen atoms, ions, and groups, and for reactions involving them (Recommendations 1988)

PREAMBLE

The names at present available for hydrogen ions or groups, and for reactions involving them, are not always adequate for describing isotopic differences. For example, the word proton is used not only for the $^1\text{H}^+$ ion but commonly, and incorrectly, for H^+ in natural abundance. In many contexts this creates no ambiguity and it is likely that this usage will continue. However, in discussions of isotope effects and in several areas of nomenclature the ability to make a distinction is essential, and the Commission on Physical Organic Chemistry recommends the terms set out below to avoid such ambiguities.

NAMES FOR HYDROGEN ATOMS, IONS, AND GROUPS, AND FOR REACTIONS INVOLVING THEM

These names comprise 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, and specific names pertaining to specific isotopes.

	General	^1H	^2H	^3H
The atom (H) ^a	hydrogen ^b	protium	deuterium	tritium
The cation (H^+)	hydron	proton	deuteron	triton
The anion (H^-) ^c	hydride	protide	deuteride	tritide
The group (-H) ^d	hydro	protio	deuterio	tritio
Transfer of the cation to a substrate	hydronation	protonation	deuteronation	tritonation
Replacement of hydrogen by a specific isotope		protiation	deuteriation (or deuteration)	tritiation

EXAMPLES

- 1 A Brønsted acid is a hydron donor and a Brønsted base is a hydron acceptor.
- 2 The observation of a protium/deuterium kinetic isotope effect may be interpreted in terms of the extent of hydron transfer at the transition state.
- 3 ^1HCl is protium chloride. K^2H is potassium deuteride.
- 4 $(\text{CH}_3)_2\text{C}=\text{O} + [^2\text{H}_3\text{O}]^+ \rightarrow [(\text{CH}_3)_2\text{C}=\text{O}^2\text{H}]^+ + ^2\text{H}_2\text{O}$ is deuteration of propanone.
- 5 $\text{CHCl}_3 + \text{C}^3\text{HCl}_3$ is tritiation of trichloromethane. The replacement of one specific isotope by another is best named ^e as, for example, in: $\text{C}^1\text{HCl}_3 \rightarrow \text{C}^3\text{HCl}_3$, tritio-de-protiation of (^1H)trichloromethane.

^a IUPAC Nomenclature of Inorganic Chemistry, 2nd edition, Butterworths, London, 1971. Rules 1.11 and 1.15.

^b The systematic name for atomic hydrogen is monohydrogen (Ref. ^a, Rule 1.4).

^c Inorganic nomenclature allows the term hydride to be used both where hydrogen is the electronegative component of a binary covalent compound and for the anion (Ref. ^a, Rules 2.22, 2.3, and 3.2).

^d This terminology is intended for use in naming transformations (Ref. ^e and other Rules in preparation by this Commission) in which the word "group" is used to describe any entity, whether monatomic or not, that may be attached to or detached from a substrate during a transformation in which it is not necessary to specify the oxidation state of the entity (compare Example 5). It is not intended that these terms should be used in structural nomenclature, for which IUPAC recommendations already exist (Ref. ^f).

^e J. F. Bunnett, *Pure Appl. Chem.*, 1981, 53, 305.

^f IUPAC Nomenclature of Organic Chemistry, 1979 edition, Pergamon, Oxford, 1979. Section H.