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[F0007]

One-Wedge Convention of Stereochemical Representation of Quadrivalent Centers

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With biographical summary

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Abstract: One-wedge convention of stereochemical representation has been introduced. We propose that the three normal bonds are imagined as bonds distributed, in a shown order

Keywords: One-wedge convention, stereochemical representation.

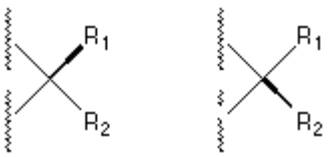
Introduction

The solid wedge, broken wedge, broken line, solid bar, and broken bar are all frequently used for structural drawing. A large number of their combinations have been seen in literature, which have caused confusion. It is clear that one type of solid wedge and only one is enough for a quadrivalent center. One-wedge convention of stereochemical representation has been introduced [1,2].

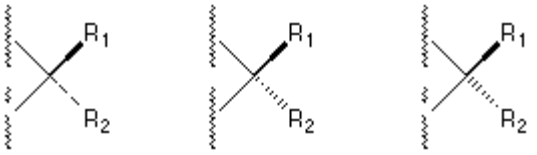
Some related recent papers and background discussions see [1-7] and papers cited therein.

Proposal of One-Wedge Convention

In a previous paper [1] we have argued that the broken wedge, broken line, solid bar, and broken bar are either not reasonable or can be replaced by only one type of solid wedge in the stereochemical formulation. A convention based on a one-wedge symbolization is proposed, where **a** or **b** is used instead of **c**, **d**, **e**, **f**, **g**, or **h.**

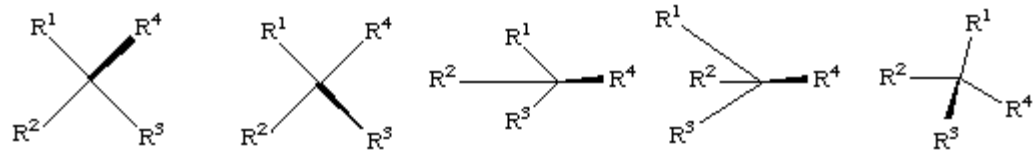


a **b**



c d e

In the original proposal [1], a restriction is made on the relative lengths of the bonds and the arrangements of these bonds. It is recognized that this restriction is not necessary [2]. We propose that the three normal bonds are imagined as bonds distributed, in a shown order, on an imaginary cone at the opposite side of the solid wedge. All the following drawings are legal and represent the same configuration.



1 2 3 4 5

Therefore, when drawing a crowded structure, some bonds can be arranged very close to each other, and some bonds may be much longer than the others, and they all still represent the same absolute configuration if the orientation of the solid wedge is the same and the three normal bonds are distributed in the same order.

Calling for Supporters' Signatures

The present author is collecting supporting signatures for the proposal of *One-Wedge Convention of Stereochemical Representation*. Please send your comments to me by e-mail during this conference and afterwards. Finally I will submit this proposal, together with the signatures of supports, to IUPAC. We also plan to test this convention [3].

Comments and Supporters' Signatures

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References and Notes

1. Lin, S. -K. A proposal for the representation of the stereochemistry of quatrivalent centres. *Chirality*, **1992**, *5*, 274-278. View this paper in html format.

2. Lin, S. -K. *One-wedge convention of stereochemical representation*, ACS 212th National Meeting, Orlando, Florida, August 25-29, 1996. Download the paper in pdf format

This proposal was also briefly presented at The First Electronic Molecular Modelling & Graphics Society Conference, October 1996.

3. This convention may be introduced in the MDPI published *Molecules* (http://www.mdpi.org/molecules/), the first electronic journal of synthetic chemistry and natural product chemistry.

4. Blessington, B. A serious problem with computer processing of stereochemistry chemical structure files: the need for standardisation. *Chirality*, **1995**, *7*, 337-341.

Dr. Blessington's contact address: Dr.Bernard Blessington . Bradford University . Dept. of Pharmaceutical Chemistry. Bradford BD7 1DP, England. Tel +44 (0) 1274 384704 FAX +44 (0) 1274 305340, e mail - b.blessington@bradford.ac.uk

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Prof. Bernard Testa, Institut de Chimie th&#65533;rapeutique, Section de Pharmacie, Universit&#65533; de Lausanne, CH-1015 Lausanne-Dorigny, Switzerland, Tel. +41 21 692 4521 / 692 4500 , Fax. +41 21 692 4525, Email: Bernard.Testa@ICT.UNIL.CH

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7. Xu, J. A proposed new convention for graphic presentation of molecular geometry and topography. *J. Chem. Inf. Comput. Sci.*y, **1996**, *36*, 25, particularly pages 31-32.

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Shu-Kun born March 24, 1957 in Hanchuan, Hubei Province, China. He graduated from Wuhan University in 1982, majoring inorganic chemistry. He studied physical chemistry in the Chinese Academy of Sciences (1982-1986, MSc in 1985) and in the USA (1.1987-7.1989). He obtained his doctorate in organic chemistry at the Swiss Federal Institute of Technology (ETH-Z&#65533;rich) in 1992 after three years studies at the group of Prof. Dr. Bernhard Jaun, Lab. f. org. Chemie-ETH-Z&#65533;rich. He then worked at Ciba-Geigy Ltd. for ca. three years, first as a postdoctoral research associate in organic synthesis and worked on two drug discovery programmes in CNS area for 1.5 years, then worked at the Dyestuffs Division of Ciba-Geigy Ltd. and received training in dyestuff R&D and production. He initiated a molecular diversity preservation project and founded MDPI (Molecular Diversity Preservation International), a nonprofit and independent international organization in Switzerland. In 1995 he launched the first journal *Molecules* that encourages authors to deposit their compound samples. He is the main author of 40 publications. He has two children (a daughter Qian-Qian, born July 27, 1986, and a son, Di-Fan, born June 1, 1996). His personal website is http://www.mdpi.org/lin.htm. Present Address: Dr. Shu-Kun Lin, Molecular Diversity Preservation International (MDPI), Saengergasse 25, CH-4054 Basel, Switzerland. Tel. +41 79 322 3379, Fax +41 61 302 8918, E-mail: Lin@mdpi.org.

Comments

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