IUPAC Conferences on Chemical Thermodynamics

A major responsibility for IACT is its involvement in the biennial IUPAC-sponsored International Conferences on Chemical Thermodynamics (ICCT). The next ICCT, which will take place 17–21 August 2004 in Beijing, China, will include symposia on electrolyte and non-electrolyte solution thermodynamics; new materials (including polymers); phase equilibria, supercritical fluids, and separation technologies; and surfactants, colloids, and interface science. A list of symposia and workshops and more information can be found at <www.ccs.ac.cn/ICCT2004.html>. The conference also features the Rossini Award and Lecture. The award is given by IACT for excellence in chemical thermodynamics.

Projects

One of IACT's principle goals is to encourage projects, particularly between different groups of thermodynamists. Following are examples of recent projects (see IUPAC Web site for details):

- Vapour Liquid Critical Properties of Elements and Compounds (K.N. Marsh; 2000-026-1-100)
- Chemical Thermodynamics for Industry (T.M. Letcher; 2002-063-1-100) (see page 17)
- Recommended values for the viscosity of molten iron and aluminium (W.A. Wakeham; 2003-005-1-100)
- XML-Based IUPAC Standard for Thermodynamic Property Data Capture and Storage (M. Frenkel; 2002-055-3-024) (see page 17)

Membership

Membership in IACT is open to all qualified applicants. Members receive a discount in the registration fee for the ICCT, are sent announcements of meetings and reports from business meetings, and are eligible to vote for the Board of Directors.

For more information, contact J. H. Dymond <Johnd@chem.gla.ac.uk>, IACT secretary.

In August, the IUPAC Council also approved the applications of the **International Plasma Chemistry Society** and the **Southern and Eastern Africa Network of Analytical Chemists** for Associated Organization status.

Inquiries about becoming an Associated Organization of IUPAC should be directed to the executive director at <secretariat@iupac.org>.

www.iupac.org/links/ao.html

Up for Discussion

A forum for members and member organizations to share ideas and concerns.
Send your comments by e-mail to <edit.ci@iupac.org>.

Questionable Stereoformulas of Diastereomers

by Gerd Kaupp and M. Reza Naimi-Jamal

Wedge bonds are still in use for the characterization of relative configurations of asymmetric centers in racemic diastereomers (e.g., in *Angew. Chem. Int. Ed. Engl.* 2003, 42, 2550). Furthermore, there seems to be an increasing misuse of such formulas as eye-catchers in graphical abstracts, when the paper itself deals with achiral compounds or racemates, but not with absolute stereochemistry or enantioselectivity (e.g., *Angew. Chem. Int. Ed. Engl.* 2003, *42*, 384; 2003, *42*, 151; 2003, *42*, 549 [does not deal with the usage of wedges in metal complexes]).

Our inquiry with journal editors points to a kind of desperate unwillingness to unify the usage of wedges for an unambiguous description of diastereomers. The violation of pertinent IUPAC recommendations prompts us to point out to the scientific community what we feel is a widespread bad habit and to urge an efficient remedy. Wedged and hatch-wedged bonds are excellent and unambiguous devices for the identification of absolute configurations in organic structural formulas. A chemical formula drawn in that manner is thus immediately attributed with *R*/*S*-descriptors by databases such as CAS/REG/SCIFINDER and stored for retrieval. There is no room for a debate that a structural formula must be correct by itself, irrespective of textural context or specifications (frequently it is not mentioned that a racemate was formed).

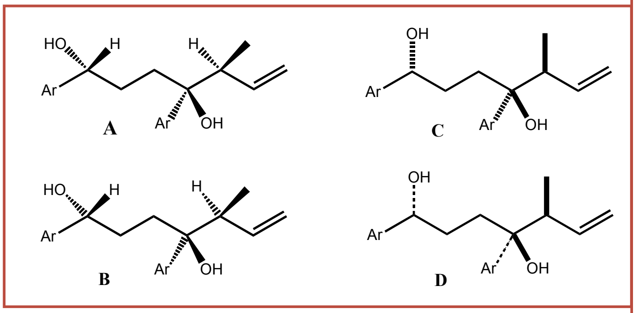
Indeed, the Beilstein database keeps with interpreting stereochemistry from the context of the formula or on its own judgment, adds and stores the word "racemate" if appropriate for its stereosearch facility not in the field "absolute" but in the fields "relative" and "racemic." However, the database adheres to the wedged formulas and this may be the reason for frequent data errors by embracing epimers under one and only one "racemate" (Scifinder also frequently does this), as can be experienced with examples from papers cited below.

If an actual racemic diastereomer is published with one single-wedged formula (e.g., in *J. Am. Chem. Soc.* **2003**, *125*, 158; *Eur. J. Chem.* **2003**, 1779; Tetrahedron **2003**, *59*, 3769; Schemes 3-5 in *Angew. Chem.* **2003**, *42*, 549), authoritative databases will at the end "pretend" absolute configurations and asymmetric syntheses. Still more disturbing is the reference of an unambiguous wedge formula to a single molecular structure image from an X-ray analysis under textual usage of starred *R*- and *S*-descriptors (e.g., [2*R**,3*R**,4*S**,5*R**] in *Angew. Chem. Int. Ed. Engl.* **1991**, *30*, 420), which are stored in the CAS/REG/SCIFINDER databases with the descriptors (2*R*,3*R*,4*S*,5*R*) (with suffix or prefix "rel"). In review articles this unambiguously formulated enantiomer may then easily appear unlabeled (e.g., in *Chem. Rev.* **2000**, *100*, 1025; on p.1048) and an absolute asymmetric synthesis is "pretended." In that situation only the application of stereochemical principles and the analysis of the reported X-ray data can unambiguously reveal that in fact a racemate had formed and not only the depicted enantiomer. Numerous problems can be envisaged.

We therefore propose to face this widespread long-term nuisance and use wedged chemical formulas only for indicating absolute configuration. Thick and hatched (alternatively broken) bonds should be used for the representation of relative configurations in racemic diastereomers, as these, contrary to the wedges, do not necessarily indicate an absolute orientation in space. They are therefore more suited for the characterization of racemates with only one formula. Enantiomers of diastereomers with known absolute configuration should always be drawn using wedges (e.g., different than the usage in *J. Am. Chem. Soc.* **2003**, *125*, 3534). The automatic recording of configurations will then easily recognize the information "racemate" or "enantiomer."

We wish to take the liberty to ask authors, referees, and editors to act accordingly in order to avoid further harm to our science. In the figure below, formula **A**, or even more distinct formula **B** (traditionally with exactly the same meaning), will then rightfully look like formula **C** (alternatively like formula **D**), if it is not the (1*R*,4*S*,5*S*)-enantiomer, but the racemate of this diastereomer.

We have noticed that some authors apparently feel the same discomfort and already draw their formulas in the suggested manner (e.g., in *J. Am. Chem. Soc.* **2003**, *125*, 761; *Eur. J. Chem.* **2003**, 1733; *Angew. Chem.* **2003**, *42*, 694).



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Response from the IUPAC Chemical Nomenclature and Structure Representation Division (VIII)

Division VIII is well aware of the problem pointed out by Drs. Kaupp and Naimi-Jamal, and will be addressing it in the course of a substantial project on Graphical Representation Standards for Chemical Structure Diagrams currently under consideration. There are published IUPAC recommendations on the depiction of stereoformulae in "Basic Terminology of Stereochemistry" (*Pure Appl. Chem.*, 68, 2193–2222 [1996]) and these will be reviewed and expanded as part of this new project.

The specific problem raised in the letter from Drs. Kaupp and Naimi-Jamal is addressed by some organisations, such as the World Health Organization, drawing the R isomer (i.e., the isomer with the *R* configuration at the lowest locant if there is more than one centre of chirality) and adding, where relevant, "or enantiomer" or "and enantiomer." There is a difficulty with the proposal to restrict the use of "thick" and "hatched" bonds to represent relative configurations, in that the reader would have no means of recognizing that this convention was being used.

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