

<http://php.indiana.edu/~davisc/Abstract.htm> (accessed Feb 10, 2004)

"NOMENCLATURE LITE:" A GUIDE TO NAMING AND INDEXING CHEMICAL COMPOUNDS

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Abstract

Chemical Abstracts index names are chosen to group items of similar interest together. They are consistent within each Collective Index period but have changed over the decades to reflect more systematic nomenclature. Although specific rules have changed, general principles prevail. These principles make it easier to choose names that promote effective communication and enhance access to information in both print and electronic form. IUPAC names may be identical or similar to CAS names, but they do not always possess implicit qualities that identify largest "parent" compounds that are more suitable for indexing. In addition, IUPAC names sometimes require locants in places that make the names more difficult to pronounce, and they may differ from CAS on the numbering of ring systems. Computers make it easier to link structures and names, but all chemists should know a few nomenclature fundamentals, especially since major journals require systematic nomenclature for publication. It is often more important to be able to name moieties within a molecule than to name the entire compound, and both IUPAC and CAS provide recognized standards that are superior to pointing and grunting.

SELECTED REFERENCES AND LINKS [excerpted from the above site]

Monographs

Chemical Abstracts Service. *The Naming and Indexing of Chemical Compounds from Chemical Abstracts*. Columbus, Ohio: 1962.

The definitive rules for CA index names. The current version, "Chemical Substance Index Names", Appendix IV of the *Chemical Abstracts Index Guide*, is now available as a reprint from CAS.

Davis, Charles H., James E. Rush. *Information Retrieval and Documentation in Chemistry*. Westport, CT: Greenwood Press, 1974.

Chapter 7 on nomenclature is the inspiration for this Web site, and provides a terse introduction to CA rules up to the 9th Collective Index. Chapters 8 and 9 treat linear notation and topological systems, respectively.

Fox, Robert B., Warren H. Powell. *Nomenclature of Organic Compounds : Principles and Practice*. 2nd ed. Washington, D.C.: American Chemical Society; Oxford ; New York : Oxford University Press, 2001.

The most up-to-date and thorough book on organic nomenclature, this work provides copious helpful examples comparing IUPAC and CAS as well as familiar (trivial) and semi-systematic names.

Leigh, G. J., H.A. Favre, and W.V. Metanomski. *Principles of chemical nomenclature : a guide to IUPAC recommendations*. Malden, Mass. : Blackwell Science, 1998.

An excellent primer and basic reference for IUPAC names with a fine chapter on polymeric (macromolecular) compounds.

Thurlow, K.J., ed. *Chemical Nomenclature*. Dordrecht, The Netherlands: Kluwer Academic Publishers, 1998.

Exceptionally well written contributions in major areas, including trivial names, natural products, and polymers among others. Interesting and entertaining coverage of history and etymology.

Software

ACD/Index Name

Perhaps the "Cadillac" of name to structure (and vice versa) software, this package, though pricey, provides for many CAS as well as IUPAC names. Templates are included for compound classes, including natural products. Educational discounts are available.

http://www.acdlabs.com/products/name_lab/

ISIS/DRAW, Autonom

Particularly useful for CAS and IUPAC ring system numbering, this package has the virtue of being available as a free download (minus stereochemistry) for those who register. Like ACD/IndexName, it has templates for major compound classes, including some natural products.

<http://www.beilstein.com/products/autonom/anm2000.shtml>

ChemDraw, Name=Struct

Brecher, J. "Name = Struct: A Practical Approach to the Sorry State of Real-Life Chemical Nomenclature."

J. Chem. Inf. Comput. Sci. 1999, 39, 943-950.

<http://pubs.acs.org/journals/jcis8/index.html>

Chemistry 4-D Draw (TM)

Includes Nomenclator(TM) and NamExpert(TM), which allow one to display a structure from a name or elicit an IUPAC name from a structure, respectively. An intuitive, responsive interface coupled with good graphics and a reasonable price help compensate for an occasional wrong name for a structure. Educational discounts are available, but be sure to get Version 6.0 or higher.

<http://www.cheminnovation.com/>

Additional Links and References from the IUB Chemistry Library

<http://www.indiana.edu/~cheminfo/14-01.html>