The Chemical Thesaurus 3.1

Robert E. Buntrock

Buntrock Associates, Inc., 11335 300th Avenue NW, Princeton, Minnesota 55371

The Chemical Thesaurus 3.1, freeware on CD, is available at the Meta-Synthesis.Com Web site, http://www.meta-synthesis.com (high-speed link highly recommended for downloading). A previous version of the software has been reviewed elsewhere.[1] Another version accompanies the paperback text by Mark R. Leach, Lewis Acid/Base Reaction Chemistry,[2] and was reviewed as part of a review of that text.[3] System requirements include a 800 × 600 monitor, 200 MB hard drive space, and either Windows 98 (or higher) or Mac 8, 9, or X. I reviewed a promotional version of the program on a CD (from Meta-Synthesis, 56 Downland Road, Brighton BN2 6DJ, UK). The program will run directly from the CD but slower than if the program is loaded onto the hard drive.

The Chemical Thesaurus 3.1 is extensively improved over previous versions intended as a supplement to a series of university level chemistry texts, Patterns in Reaction Chemistry. The texts are noteworthy in that there is no distinction between organic and inorganic chemistry. As a thesaurus, the Chemical Thesaurus 3 (henceforth CT3) is more like a "classic" thesaurus—a treasury or storehouse—rather than the hierarchical thesauri used for information retrieval (e.g. MeSH from the National Library of Medicine used for indexing and searching MEDLINE). Of course, CT3 accomplishes its tasks by extensive hyperlinks between several databases and their contents.

The thesaurus itself consists of 4 parts: Chemical Species, Sorts & Finds, Chemical Reactions, and Reaction Searches. The Chemical Species portion is an alphabetic synonym list of chemical entities. Clicking on a listing links the user to a detailed data sheet including structure, names, molecular formula, and properties (mp, bp, density, and solubilities). Clicking on the reactions box ("... processes from ... as a substrate or reagent") produces a list of reactions. Clicking on the products box ("... processes from ... as a product") lists reactions producing the compound. Some industrial processes are included in both.

For example, clicking on acetaldehyde yields a typical display with 11 reactions and 17 preparations. The preparations include 2 retrosyntheses plus oxidations or hydrations either catalytic or otherwise facilitated by metallic species. Scrolling down to the syngas (synthesis gas) → acetaldehyde preparation and clicking on the arrow yields a description of syngas as a mixture of carbon monoxide and hydrogen. Clicking on the accompanying box "organic industrial processes" yields additional organic industrial processes.

Clicking on the reactions box yields 11 reactions including one of the retrosyntheses described above, plus the aldol condensation and a three step industrial preparation of 1,3-butadiene from acetaldehyde. Clicking on the triple arrow (indicating 3 step) yields a description of each of the steps.

Going back to the Chemical Species list and clicking on acetaminophen produces a screen with structure, names, properties, preparations, and no reactions. Additional links include analgesics and biologically active substances. Clicking on the former yields two analgesics, aspirin and acetaminophen. Clicking on the latter yields several additional compounds and classes of compounds.

Clicking on terephthalic acid (1,4-benzenedicarboxylic acid) yields 2 preparations—the Amoco and Henkel oxidations of *p*-xylene—and 2 reactions, both polymerizations to produce PET (poly(ethylene terephthalate)).

Mixtures and substances of indefinite composition are included. Clicking on naphtha yields a screen with the description, "mixture of C_6−C_{10} hydrocarbons". The preparations described include crude oil → naphtha and gas oil with hydrogen and zeolite catalyst → isobutane, gasoline, and naphtha. Reactions include naphtha → various olefins. Clicking on any of the species yields further information and data on that species.

Clicking the "Sorts & Finds" box on the Main Menu yields a page where sort or find operations can be performed by full or partial name, contained element, or a list of various categories. One of these categories is "spectra". A few listings have IR or NMR (H or C13) and more spectra will be added in the future.

The Chemical Reactions Box on the Main Menu is a list of all reactions in the databases, arranged alphabetically by the key substrate. The list is also sortable by 1st reagent, 1st product, or 2nd product.

The Chemical Reaction Search Box allows reaction searching by 15 categories (including name reactions) and 5 broader categories (including biosynthetic or industrial chemical reactions). There are 12 name reactions found by clicking "name reactions", including Diels−Alder cycloadditions.

In addition to these 4 primary boxes on the Main Menu Thesaurus, there are a list of "gadgets" and "extras". Gadgets include a periodic table, a molecular weight chart, and descriptions of redox chemistry, aromatic substitution, and thermochemistry.

The periodic table can be displayed "plain" or with the appropriate elements highlighted per a number of categories. These include among others, groups, either current or previous IUPAC; group numbers 1−18, biological status (including essential, essential trace, toxic, or radioactive), electronegativity, material type, and superconducting. Clicking on the element on the chart yields a complete data sheet for the element.

The thermochemical gadget lists several reactions with thermochemical data. For those listed, the temperature can be adjusted to produce a change in the delta G of the reaction.

The extras include a reaction chemistry tutorial and a glossary. The latter contains a list of both symbols and terminology. For example, ⟹ is defined as retrosynthetic, and "synthon" is defined as a synthetic equivalent in retrosynthetic analyses.

Overall, I believe this is an excellent program for support of a number of college chemistry courses. Although not as comprehensive as many chemical reactions databases, it might even be useful to postgraduates as a primer or "jump start" to gain access to an unfamiliar or forgotten area of

chemistry. All data and information is extensively linked and is fairly easy and logical to navigate. However, I would prefer a "back" button, which is intentionally omitted. Although the author would prefer users to "go forward", there are times when browsing leads to a blind alley or less interesting results. In these cases, it would be easier to navigate if one could back out into a previous list and explore another branch without being required to start over.

REFERENCES AND NOTES

(1) Cousins, K. R. *J. Am. Chem. Soc.* **2001**, *123*, 8645−6.
(2) Leach, M. R. *Lewis Acid/Base Reaction Chemistry*; Meta-Synthesis-.Com, Brighton, UK, 1999. 95 pp. Figures, tables wall chart, and CD-ROM tutorials.
(3) Cochran, J. C. review of *Lewis Acid/Base Reaction Chemistry*. *J. Chem. Educ.* **2001**, *78*, 166.

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