COMPUTER SOFTWARE REVIEWS

The Aldrich Catalog on CD-ROM

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Received January 25, 1993

To a chemist, the *Aldrich Catalog Handbook of Fine Chemicals* is a valuable reference work, worth keeping close at hand and often used. Students in organic chemistry laboratory, prior to carrying out their experiments, list in a preliminary writeup the reagents involved and their properties, and the *Aldrich Catalog* is recommended as the first place to look (try finding pyridinium perbromide, 2-methyl-3-butyn-2-ol, or norbornenedicarboxylic acid in the CRC or *Lange's Handbook*; yet these are the compounds in everyday use in an undergraduate lab, and their properties are needed before the experiment can be started). A chemist who runs a reaction and needs to buy a reagent reaches for the *Aldrich Catalog* first, and only occasionally needs another source for a reagent not sold by Aldrich, or cheaper, or in a more convenient size (usually cheaper) than in the *Aldrich Catalog*. If you are interested in an infrared or NMR spectrum, the *Aldrich Catalog*, with its references to the Aldrich spectral collections, is a very handy place to look for a spectrum of a compound or an analog. During an online search it is often necessary to find a CA Registry Number quickly!, and if the compound is sold by Aldrich, the *Aldrich Catalog* will give it. We keep copies of the *Aldrich Catalog* at several strategic locations in our Science Library.

So we approached the *Aldrich Catalog on CD-ROM*[1] from several points of view—as a handbook, where a student might look for data, as a catalog, where a research chemist would look for reagents, and as a database for other information.

The CD-ROM Catalog, which includes the 31 000 chemicals in the *Aldrich Catalog*, also includes at least a large number of the (37 000) chemicals in the ABC Library of Rare Chemicals, chemicals available in small quantities, which are not listed in the regular catalog.

The disk installation was routine. The disk is accompanied by a small instruction manual, which is occasionally of use even after the simple search technique is grasped.

Our installation was on a computer with a mouse. Commands from the menu bar at the top of the screen can be moused, or the first letter will activate them (occasionally—during several uses there was no response to the letters). Activating the **search** command brings down a menu with choices for *Aldrich Catalog* number, name, formula, and CAS registry number. The choice can be moused or initialed, to give a window for data entry. The instruction manual suggests that a name can be searched with or without substituent numbers (**dichlorobenzene** or **1,2-**, **1,3-**, or **1,4-dichlorobenzene**). However, a search for **methylbutynol** gave a response that there was no entry. Since we knew the compound was there, several modifications were tried, all with a negative response. Finally, the catalog was consulted for **methylbutynol**, and the entry was found as **3-methyl-1-butyn-3-ol**. Searching for **3-methyl-1-butyn-3-ol** retrieved a name menu. The next candidate was palladium on charcoal. **Palladium** got a negative response, as did **pd1** as a formula. Eventually the *Catalog* suggested **palladium on carbon**, which brought up the name menu, with several choices for various Pd/C catalysts. Generally, it was easier to look in the *Catalog* for a name search, since *Catalog* entries are alphabetized without considering substituent location numbers.

Another disconcerting feature of name searching is the inconsistency in nomenclature. **2-Methylpentanoic acid** gets a negative response (no compound name menu is presented)—the name is **2-methylvaleric acid**; **2-methylvaleric hydrazide** gets a negative response—the name is **2-methylpentanoic hydrazide**. Similarly, **methanephosphonic acid** retrieves nothing, **methylphosphonic acid** does, but **methanephosphonic acid dimethyl ester** is necessary for the synonymous **methylphosphonic acid dimethyl ester**. In short, it is almost necessary to have the *Catalog* at hand to use the CD.

On the positive side, the structures are beautiful, the structure for buckminsterfullerene particularly impressive (except for a circle, probably used as a template, around the C_{60} drawing). On the negative side, many of the structures are messed up, apparently one atom gets covered up by another, and a substituent appears attached to a wrong atom (for example, 2-methylvaleric acid, 2-methylvaleric hydrazide, 3-methylvaleric acid, and many others).

Other positive features of this product are the legible formulas (the miniscule subscripts in the *Catalog* formula index are almost impossible to read without help), and the references to the Aldrich collections of infrared and NMR spectra (although the line dedicated to (two) IR maxima seems wasted), Fieser's *Reagents* (limited to eight entries, apparently not always the latest eight), and the *Merck Index* (latest edition), and the inclusion of compounds from the rare chemicals catalog, available in small quantity.

Since a catalog is used when reagents are purchased, this aspect of the database was also of interest. From the compound screen a price list can be called up (**Add to P/O**, from the pull-down Miscellaneous menu). However, this selection cannot be activated until a Purchase Order is initiated (from the File menu). This is a moderate annoyance, requiring the File pull-down menu, selection of **New P/O**, and two data entry screens (the file must be named for the P/O to be opened). Once this is done the price list can be called up. However, there may be many entries corresponding to a single Name retrieval, for example 19 entries for acetone. If **acetone** was retrieved from a Name search, and the first entry retrieved from the name list, it is not possible to return to the name list window to examine the other entries. Using Page Down will retrieve the next entry from the list, but if you are in the price

list and decide to look at prices for other choices, Page Down does not work—you have to Escape to the compound entry, Page Down to the next entry, select **Miscellaneous** and **Add** to get the price list, and decide if this is any better. This is an extreme example, but not a rare one—benzylmagnesium chloride has three entries, not differing by isotopes as some of the acetone entries are. It seems to us that for a chemist interested in economy, the *Catalog* is much handier.

The Print command prints a very handsome order, from the P/O assembled above (single items can be easily deleted). This seems to be not of great use, since the toll-free telephone order number offers instant availability information as well as an instant purchase order.

A few more nits are left to pick. The dedicated arrow, Home, End, and Pg Up/Pg Dn keys do not function, the keys from the number keypad (with Number Lock off) must be used, but these keys are much handier than the top row when a moderate number of digits are to be entered. Also, from a name list it is often useful to Page Up or Page Down to continue the list, but the new page is not highlighted, so the arrow keys do not function—it was only after much frustation that it was found that the space bar will cause highlighting of the top name, and then the arrow keys work.

One tantalizing feature of the pull-down menus are selections that are not active (in light gray letters), such as Name Fragment and Substructure in the Search list. These apparently are active in the ALDRICHEM Data Search product (at $495.00).

All things considered, although this product is moderately priced ($25), it will not replace the hardcopy, annually revised *Aldrich Catalog Handbook of Fine Chemicals*. Some modifications that would make it more convenient to use would be the ability to return to the compound name menu after an item has been selected, eliminating numbers from the compound name alphabet, and access to the price information without opening a purchase order. It would also be of value if the display screen could be printed.

REFERENCES AND NOTES

(1) *Aldrich Catalog on CD-ROM*, Aldrich Chemical Co.: St. Louis, MO; Cat. No. Z20,446-3 ($25.00). Corresponds to *Catalog Handbook of Fine Chemicals, 1992–1993* published by the same company. System requirements: CD-ROM drive, DOS ≥ 3.1, 640K RAM (512K available), Hercules monochrome or CGA, EGA, VGA or MCGA color graphics, hard disk or 2 diskette drives.