COMPUTER SOFTWARE REVIEWS

CRC's *Properties of Organic Compounds* CD-ROM

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Property data are valuable to both the student of chemistry and the researcher. CRC Press has produced a single CD-ROM called *Properties of Organic Compounds*, a database of properties for over 27 000 organic compounds.[1] Although not stated specifically in the documentation, it seems to be based largely upon data in the *Handbook of Data on Organic Compounds*, 2nd ed., published by CRC Press.[2]

This CD-ROM requires an IBM PC or compatible with an 80386 microprocessor or higher, 2 MB RAM, 2 MB hard drive disk space, a VGA monitor, a high-density disk drive (3.5 in. or 5.25 in.), a CD-ROM drive (usually Hitachi, Phillips, or Sony) with Microsoft Extensions (MSCDEX) version 2.0 or higher, and Microsoft Windows version 3.1. For the purpose of this review, it was installed on an IBM 80486 PS/ValuePoint with a VGA monitor, 6 MB RAM, 170 MB hard drive, an external Hitachi CD-ROM drive, and an Okidata Microline 590 (24-pin) printer.

The following properties/data can be found in *Properties of Organic Compounds*: Beilstein Reference, CAS Registry Number, boiling point, melting point, molecular weight, density, color, refractive index, solubility, specific rotation, and spectral peaks (mass spectra, Raman, ^{13}C NMR, ^{1}H NMR, infrared, ultraviolet). References are included for the spectra data. Searches can be performed on ranges and/or combinations of properties (boiling point, melting point, density, molecular weight), chemical name (as well as synonyms), molecular formula, spectral peaks (listed above), and CAS Registry Number.

This CD-ROM comes with a 43-page user's guide, as well as a ready reference card to be kept nearby for searching. A separate page of "software notes" contains additional information that is not in the user's guide. On-line help is available by clicking the help button (with the "?" symbol). The help facility is context sensitive. The majority of the text of the user's guide is in the on-line help screens and can be searched and/or printed at any time. I found this to be much more useful than the user's guide, which had a table of contents, but no index.

The installation of the software is straightforward. The software directs Windows to create an icon called "Properties of Organic Compounds" and a group window called "CRC". The title screen is programmed to display in 30 s. This is somewhat annoying and can be overridden by clicking the mouse once. A small glitch occurred during the installation when I attempted to use the help button at the system configuration window. The message "Cannot open Help file" appeared. Obviously, the help files were not loaded at that time. Once I moved to the main window, however, the problem no longer occurred.

The user of this CD-ROM needs to know how to get around in Windows using the mouse to "point and click". However, if one has problems with the mouse, keyboard equivalents are listed in an appendix in the user's guide.

The main window of *Properties of Organic Compounds* has seven different buttons: five for each of the different types of searches (name, molecular formula, CAS Registry Number, properties, and spectral peaks), one for on-line help, and one for "File" operations.

In general the searches are easy to perform, if one follows the on-line directions. Once a search is performed, identifying information from all records matching the search criteria appears in the retrieval window. The searcher then highlights the record to view and clicks the View button for the data and structure, if present, of the associated compound. The scale of the structure can be adjusted when setting the system configuration or upon viewing.

The name search does not require the exact CAS index name, which is displayed in the data window. One can search on synonyms, trade names, and abbreviations. Since this CD-ROM does not support structure searching, this feature is quite useful. The search engine requires that one leave out numbers, spaces, punctuation, and special characters and character strings when entering any compound name, even the CAS index name. Both upper and lower case letters can be used. For example, both "MEK" and "methylethylketone" will retrieve the record for "2-butanone". Perhaps future versions of the search software will have code to remove these "superfluous" characters for the searcher. The chemical names for all matching records are listed in the retrieval window. It would be helpful if synonyms could be grouped together in this window or if all synonyms could be listed with the compound data.

Atoms of a molecular formula can be entered in any order without spaces for a search. The letters must be upper case, except for examples like the following: "Cl" for chlorine and "Co" for cobalt so that there is no misinterpretation, say of "co" for carbon and oxygen. The retrieval window displays the compound names for matching records.

Property searches can be performed on single values, ranges, and Boolean combinations of properties. The properties and operators are selected from a list of options, and the searcher is prompted to supply a value or range of values. The length of time for a property search can vary widely, depending upon the complexity of the search and the number of matching records. Property data, CAS Registry Number, and the compound name for each matching record appears in the retrieval window.

Spectral peaks can be searched. Once the spectra type (mass spectra, Raman, ^{13}C NMR, ^{1}H NMR, infrared, ultraviolet) is selected, peaks can then be entered separated by either spaces or commas (but not both). Peak data for each retrieved record are displayed in the retrieval window.

I encountered some problems when attempting to view and print the data. Most of the compounds that I retrieved did not have a structure. I almost missed the first record with a structure because the structure window was almost totally off the screen. The leftmost edge of the structure window

appeared at the far right of the screen. Using the mouse, I had to "drag" the structure window over to the center of the screen, under the data window. I then used the mouse to click to the screen, either data or structure, that I wished to view. Both the data and the structure can be copied to a file (in "Rich Text Format" with a DOS file extension of rtf) or to the Windows clipboard for direct copying into another Windows application running concurrently, or it can be directly printed. With the print option, some special characters do not print as they appear on the screen. The software does not have any special printer configuration, so this small problem was not surprising. When attempting to print the data on some sugars, matching on "glucose" and "sucrose", I encountered an error condition "Illegal function call". After I clicked the window, the program terminated, and I was returned to the Windows Program Manager. WordPerfect for Windows version 5.1 was able to read the data portion of the "rtf" file and convert it to proper fonts and special characters, but it did not convert any of the structure data. When a structure is printed, a "gridlike" background is also printed. This interfers with the quality of the structure.

After selecting "Close Form" at the data window, the system requires several steps to return to the retrieval window to select other records: click on "File", select "Window", and then select the specific category of search to recall. This is awkward. It would be easier if one could select to return to either the main window or the most recent retrieval window.

The technical support personnel at CRC Press for this product were courteous and responsive to my questions on the file and print problems. They quickly identified the cause of the error condition that I encountered with printing data from some of the sugar compounds and said that they would correct it in the next release of the software.

There are two other CD-ROMs of chemical properties that I am aware of, the *Aldrich Catalog on CD-ROM* and the *CHCD Dictionary of Organic Compounds* on CD-ROM; however, I have no direct experience with either. According to the sales literature, both of these titles cover more compounds, and the latter title has structure searching capabilities.

The *Properties of Organic Compounds* CD-ROM differs from the above titles in that it contains spectral peak data, not just references to spectral data. The costs of this CD-ROM and of the *CHCD Dictionary of Organic Compounds on CD-ROM* are comparable. However, this CD-ROM can be networked for up to 10 users with no additional cost, which might make it feasible for networking to workstations in teaching laboratories and a science library. The very high cost of this reference is questionable if printed sources have already been purchased, as they are in my library, or if there is ready access to on-line databases, such as *Beilstein Online*.

REFERENCES AND NOTES

(1) Properties of Organic Compounds, a CD-ROM, has a list price of $2795.00.

(2) *Handbook of Data on Organic Compounds*, 2nd ed.; CRC Press Inc.: Boca Raton, FL, 1989.