COMPUTER SOFTWARE REVIEWS

ChemWindow Release 3 and ^{13}C Module

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ChemWindow (Softshell International) is a Windows-based, chemical drawing program. Graphics can be created and manipulated quickly and easily with ChemWindow (using a palette of drawing tools) and can be imported into most popular word processing programs. In addition, ^{13}C chemical shifts can be predicted for structures created with ChemWindow using the optional ^{13}C module. This program has numerous, well-integrated features which provide significant flexibility and useability.

SYSTEM REQUIREMENTS AND INSTALLATION

The recommended minimum system configuration for running ChemWindow is as follows: Microsoft Windows 3.1, a 386 (20 MHz) or higher processor, 4 MB of RAM, a hard disk, and a mouse. ChemWindow will, however, run under Microsoft Windows 3.0 if an appropriate type manager is also installed. The additional ^{13}C module requires Release 3 of ChemWindow and cannot be used with earlier releases. Finally, a Macintosh version of this program (ChemIntosh) is also available, but will not be reviewed here.

Complete installation (which I was able to do without opening the manual) of ChemWindow and the ^{13}C module required approximately 2.8 MB of hard disk space. It should be noted that this review of ChemWindow was performed on a 486DX (33 MHz) machine with Microsoft Windows 3.1, MS-DOS 6.2, 8 MB of RAM, and a local-bus, Windows-accelerator video card. I did have some difficulties, however, with ChemWindow and Windows video drivers. Initially, I was using an 800 × 600, 256 color Windows video driver that was supplied by the manufacturer of my video adapter. I had not experienced any trouble with this particular driver until I started using ChemWindow. I received several, sporadic Windows "General Protection Faults" (which corrupted the application) while I was using ChemWindow and the manufacturer's driver. In fact, the ChemWindow documentation lists several video adapters that are known to cause problems with ChemWindow (mine was *not* on their list). I called SoftShell to see if I could obtain an updated driver for my particular video board (as suggested in the ChemWindow documentation), but the driver for my adapter was not available.

There were two solutions recommended by SoftShell for the video driver problem. First, small bitmapped images can be employed that solve the Windows problems with some video drivers. For example, if the control key is depressed when ChemWindow is started, a "Startup Settings" window is obtained where small bitmapped images can be selected. This option had no effect on my system, and I continued to receive "General Protection Faults". The second alternative was to use the Microsoft Super-VGA (SVGA, 800 × 600, 16 color) video driver that is supplied with MicrosoftWindows 3.1. I have not had any problems with ChemWindow since I switched to this video driver.

NEW FEATURES

There are several new features and improvements in Release 3 of ChemWindow. First, a "chemical syntax checker" has been added which will "proofread" chemical structures. If the syntax checker discovers an error, the point at which the error was found is displayed, and the structure can then be modified appropriately. Second, atom labels can be entered much more easily than in previous releases. For example, a Periodic Table has been added in addition to "hot keys" which can be used for common atom labels (e.g., CH_3, NH_2, OH, etc.). Third, a cross-hair tool has been added which can be used for aligning graphics. Fourth, the "make stick structure" tool can be used for converting structures that have been drawn using atom labels (e.g., CH_3, C_2H_5, etc.) entirely to stick-structures. Finally, a pen-tool for drawing lines, curves, arcs, etc. has also been added.

USEABILITY

ChemWindow is extremely easy to use. Graphics are created by selecting drawing tools from a palette. The palette contains tools for drawing most types of bonds and rings, manipulating and aligning objects, and drawing various symbols, text, and atom labels. I found that the most important attribute of ChemWindow was the speed with which structures could be drawn. Very complete structures could be created in seconds by simply "sprouting" bonds and rings. The Periodic Table and the atom label hot keys also increase the speed with which labels can be created. Finally, the ability to "undo" more than the last operation saves much time and effort.

There are a variety of drawing "styles" (i.e., a collection of adjustable parameters for selecting the size, width, font, etc. for each type of drawing tool) that are included with ChemWindow. However, styles can easily be created or modified to suit the user's needs and preferences. There is also an album/template tool which allows the user to retrieve commonly-used structures or graphics that were previously saved in an album or template.

Several of the new features in Release 3 add significant flexibility to the program. The chemical syntax checker gives the user the option of either correcting the error or "teaching" the program that the "error" is acceptable and to ignore it in the future (these modifications to the valence rules are saved in a disk file). Second, the "make stick structure" tool converts structures that include atom labels

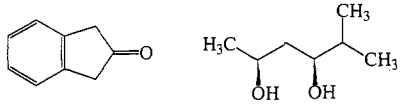

Figure 1.

entirely to stick structures. Although I do not believe that I would use this tool very often, its availability would save a significant amount of time in those instances when I needed to perform such a conversion.

ChemWindow can export several different types of file formats: (1) Word Perfect Graphics (WPG), (2) Windows clipboard and metafiles, (3) encapsulated PostScript (EPS), (4) ChemDraw 2.*x*, and (5) MDL molfiles. I was able to import structures into Word Perfect for Windows 6.0a (Word Perfect Corp.) via the Windows clipboard quickly and easily.

The printed manual that is supplied with ChemWindow as well as the on-line help within the program are both verygood and well-organized. In addition, the quality of the printed output is excellent. For example, the structures shown above were created using the "Presentations" style which is included in ChemWindow. These structures were printed on a Hewlett-Packard LaserJet III using a PostScript cartridge.

^{13}C MODULE

The ^{13}C chemical shift algorithms incorporated into the ^{13}C module of ChemWindow were developed by Dr. Erno Pretsch and Andras Furst at the Swiss Federal Institute of Technology (see: Furst, A.; Pretsch, E. *Anal. Chim. Acta* **1990**, *229*, 17. Furst, A.; Pretsch, E.; Robien, W. *Anal. Chim. Acta* **1990**, *233*, 213. Furst, A.; Pretsch, E.; Robien, W. *Anal. Chim. Acta* **1991**, *248*, 415. Pretsch, E.; Furst, A.; Badertscher, M.; Burgin, R.; Munk, M. E. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 291.). I computed the ^{13}C chemical shifts for 56 compounds (322 total carbon atoms) selected from the literature. I attempted to construct a representative sample by selecting acyclic, cyclic, and bicyclic molecules which contained various types of functional groups. The average error (per carbon atom) for this set of compounds was 4.3 ppm, although errors as large as 21−23 ppm were also obtained. Even though the predicted ^{13}C chemical shifts were not always accurate, the trends were generally qualitatively correct.

Several points about the ^{13}C module should be mentioned. First, the module can properly treat geometrical isomers but *cannot* treat stereoisomers or charged species. Second, structures that contain atom labels (e.g., CH_3, C_2H_5, etc.) are automatically converted *entirely* to stick structures before the ^{13}C analysis is performed. I found this to be particularly annoying because it was then necessary to edit the structure to replace the original atom labels. Finally, the predicted chemical shifts are often placed (as a single object) too close to the respective carbon atoms which makes them difficult to read. I found it necessary to move the chemical shift data away from the molecule to accurately read the values.

PRICING

The single-user price for ChemWindow Release 3 is $599 ($399 academic). Students can purchase a single-user copy for $99. This price does *not* include the ^{13}C module which is an additional $99. ChemWindow comes with a 30-day, money-back guarantee, free technical support, and periodic newsletters.

SUMMARY

Despite a few minor problems, ChemWindow is the best chemical drawing package that I have used. Drawing complex chemical structures is quick and easy, and the quality of the printed output is excellent. SoftShell has clearly made a dedicated effort to make ChemWindow *easier* to use than previous releases. Moreover, the optional ^{13}C module should be a useful addition for both student and researcher. Even though the single-user price seems somewhat steep, ChemWindow, overall, is an excellent software package.