CS ChemDraw Pro,[1] Version 3.1 for Windows

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CS ChemDraw is Cambridge Scientific Computing's (CSC) chemical structure drawing program. It is distributed in two versions, ChemDraw and ChemDraw Pro, formerly called ChemDraw Plus. Both programs are full-featured chemical drawing programs, but the Pro/Plus version includes some additional features: user-definable template documents, color capability, and a wider selection of export and import formats. The software reviewed is the first release of ChemDraw Pro in a Windows-compatible version after 7 years as a Macintosh application.

The software requires a 386 or higher PC with at least four MB RAM. In addition, CSC recommends at least 5 MB of virtual memory. I tested ChemDraw Pro on both a 25 MHz 386 PC with an 80 MB hard drive and a 50 MHz 486DX PC with a 450 MB hard drive. Each computer had only four MB of RAM. Furthermore, the small amount of free space which remained on my 386 PC's drive was very fragmented. Consequently, Windows was unable to reserve the recommended virtual memory, and its performance suffered. In spite of this, the software performed adequately, although slowly, on that platform. Because I intend to use this program mostly to prepare figures for export into a word processing program, most of my tests were done with both ChemDraw and WordPerfect for Windows active. As expected, the operations were all slower under those conditions—painfully so with the 386 PC. While performance was satisfactory on the 486 with 4 MB RAM, I would recommend 8 MB to anyone planning to use ChemDraw and another application, especially a word processing program, concurrently.

With the 486 PC, but *not* the 386, I occasionally encountered memory management problems when using ChemDraw. According to Cambridge Scientific, these problems are due to incompatibilities between Microsoft's WIN32s, supplied with ChemDraw, and some computer configurations. Following CSC's suggestion, I recently updated WIN32s to Version 1.15a, available by FTP from Microsoft. The memory problems have not recurred.

I found ChemDraw Pro to be very easy to install and use. The *Quick Start Tutorial* in chapter 1 of the User's Guide will be sufficient training for most users of this software. Using it as my only training, I was able to use most of the structure and text drawing tools within an hour of opening the package. I expect that the same will be true of anyone familiar with Windows and the use of a mouse. The tutorial is also available as part of the on-line help, but I found that less useful because the help window disappears each time the tools window is selected!

STRUCTURE DRAWING

Drawing structures in ChemDraw is accomplished by the *click* and *drag* operations familiar to Windows users. To begin a figure, one simply selects the appropriate bond or other structural features from the "Tools" window and deposits it in the document by clicking or dragging the mouse. Bonds can be added to an existing structure or changed by clicking at the appropriate location in the figure. Double and triple bonds are generated by draging the second and third bonds between the appropriate atoms. The ChemDraw Tools window includes a wide selection of structure drawing tools. Besides ordinary bond lines, dative, bold, hatched, and wavy bonds and solid, open, and hatched wedges are available. The menu also includes benzene, cyclopentadiene, common (three- to eight-membered) alicyclic rings, cyclohexane chairs, and a very useful acyclic chain tool. The latter allows one to draw a long chain of atoms simply by dragging the mouse until the desired chain length is drawn. Finally, the Tools window includes eight sets of structure templates containing over 200 additional structure elements. Each of these can be added to the figure with one mouse operation. Each template can be used as the basis of a figure or incorporated into an existing figure by clicking a bond or atom. Other structure drawing programs include templates; none I have used offers direct access to as many structures. ChemDraw Pro, but not ChemDraw, also allows the user to create custom template documents and to edit existing templates.

INCORPORATION OF TEXT AND OTHER DRAWING ELEMENTS

Incorporation of text, either in atom and group labels or in captions, is accomplished easily in ChemDraw. A single "smart" text tool allows one to add atom or group labels to structures or to add captions to figures. Text added at the end of a bond is recognized as an atom or group label and automatically formatted to render numbers as subscripts. When the text is not at the end of a bond, the tool recognizes it is writing a caption and uses normal text for letters and numbers. Both *label* and *caption* text formats can be set by the user and overriden easily if necessary. An additional convenience of ChemDraw is its ability to add labels without selecting the text tool; double clicking the end of a bond while a drawing tool is selected allows entry of a label without leaving the drawing tool.

Besides the structural elements, the ChemDraw Tool window includes common reaction symbols and a variety of arrows, including reaction, equilibrium, resonance, retrosynthetic, and "electron pushing" curved arrows. A selection of orbitals, a selection of other drawing elements, such as boxes and brackets, an arc-drawing tool, and a very good curve drawing tool complete the menu. I particularly liked the curve tool, which was easier to use and more versatile than others I have encountered.

CUSTOMIZING FIGURES

One of ChemDraw's strengths is the ease with which it can be customized. The *Preferences* and *Options* menus allow the selection of all characteristics of the structures, including bond length, the angle between adjacent bonds, line thickness, and many other features. One can also select the font, size, and style of atom labels and captions. These settings can be saved as a "style document", which can be recalled whenever preparing figures for the same purpose. Changing all of the settings can be accomplished simply by selecting the appropriate style document. This is a much more convenient operation than changing every setting in the preferences and options menus. ChemDraw comes with several of these style documents, including settings for *Synlett*, the journals of the Royal Society, and the *Journal of Organic Chemistry*. Unfortunately, the *J. Org. Chem.* settings are those specified in the 1993 *Instructions to Authors*; the 1994 specifications are different, although both produce the same size figures.

The ability to define ones own style documents and to create sets of templates makes it very easy for each user to customize ChemDraw for a specific application and to switch among styles. Since these settings are stored in easily-loaded style and template documents, switching is a simple matter of choosing the appropriate style when the document is opened.

EXPORTING AND IMPORTING FIGURES

Chemical drawing programs are often used to prepare figures for export to other programs and to edit drawings produced by other applications. It is important, therefore, that the drawing program is able to import and export files in a variety of formats. In addition to its native format (*.CHM), ChemDraw can open and interpret MDL MOL-files, Molecular Simulations MolFiles, SMD files, and connection tables. It also will save documents in these formats as well as PostScript, SMILES, and Windows Metafile documents. Figures can be transferred to and from ISIS/Draw by saving and then importing them as MOL files. HyperChem structures saved as MOL files can also be imported into ChemDraw, appearing exactly as they did on the HyperChem screen. Once in ChemDraw, the structures can be edited as native ChemDraw figures. The reverse operation cannot be accomplished without extensive editing of the ChemDraw MOL file; several columns of zeroes are missing.

Incorporation of ChemDraw figures into a word processor document is most conveniently accomplished by cutting and pasting them using the Windows Clipboard. The figures can also be cut from the document and pasted back into ChemDraw for editing. ChemDraw suggests exporting figures to word processing documents as Windows metafiles (*.wmf), but I found that method unreliable and cumbersome. Saving *.wmf files can be very slow, and ChemDraw cannot read and interpret figures saved as *.wmf files. Of greater concern is the fact that occasionally some atom labels disappeared, both from the *.wmf file and the active document, during the *save* operation![2] For all of these reasons, the cut and paste operation is preferable whenever it can be used.

DOCUMENTATION

Documentation for ChemDraw includes the User's Guide and the release notes included in a README.TXT file. Both are written clearly, with few significant factual errors. As I mentioned above, the *Quick Start Tutorial* in chapter 1 of the User's Guide is well done, giving the beginner practice with most of the features of ChemDraw. Because most of the Guide is organized by tasks, it was very easy to find more detailed descriptions of any ChemDraw operation. Perhaps to be expected in a first printing, there are several errors in the Users' Guide. Most are typographic errors that a spell-checker would not detect, such as "draw" instead of "drag", and "form" instead of "from". The authors also incorrectly name the product of the reaction in the tutorial. I found only two substantial errors. Once in the introduction and once in the tutorial, the functions of the *control* and *alt* keys are interchanged. In another section, the Guide indicates that clicking in an empty space when the curve tool is selected will deselect an existing curve. When one performs this operation, the action will draw a second curve at the point clicked! In spite of these troublesome errors, the User's Guide is very helpful and easy to use. The typographical errors and the incorrect name are distracting but not misleading, and the errors in the use of the commands appear only once each. Since the commands are described and illustrated correctly in the remainder of the Guide, the errors are not likely to lead to significant difficulties in using the software.

CONCLUSION

I consider ChemDraw for Windows a welcome addition to the list of chemical drawing programs for Windows. It is a powerful chemical structure drawing program with many outstanding features and few weaknesses. Its tools make structure generation very easy. Its user-definable template and style documents allow each user to customize ChemDraw and place numerous drawing styles literally at ones fingertips. It can import and export structures in a variety of formats, making the transfer of structures to other applications very easy. Its major weaknesses are memory errors on certain computers, the unreliability with which it saves *.wmf files, and some errors in the documentation. Upgrading the WIN32s files seems to have remedied the most serious of these, the memory handling problems. In spite of these few weaknesses, I was very impressed with ChemDraw for Windows and plan to use it as my principal structure drawing program.

In its Macintosh version, ChemDraw is part of a suite of programs called ChemOffice. This package also includes Chem3-D, a molecular modeling program, and ChemFinder, a chemical database. Based on my experience with ChemDraw for Windows, I am looking forward to the release of the remainder of ChemOffice in a Windows version.

REFERENCES AND NOTES

(1) ChemDraw Pro and ChemDraw, Cambridge Scientific Computing, Inc., 875 Massachusetts Avenue, Cambridge, MA 02139.

(2) CSC is aware of this difficulty; it is described in the release notes on the program disks.