ChemOffice Plus: A Package of Programs for Chemists

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CSC ChemOffice Plus for the Macintosh computer includes three programs, CSC ChemDraw Plus 3.0.2, CSC Chem3D Plus 3.1.1, and CSC ChemFinder 1.1.[1] According to the promotional literature, CSC ChemFinder "seamlessly integrates searching by structure and other criteria with the drawing tools of CSC ChemDraw and the modeling features of CSC Chem3D." ChemFinder uses folders of molecules as a database that can be searched the way chemists think: by name, by molecular formula, or by two- or three-dimensional structure. A two- or three-dimensional structure can be entered easily into a new or existing folder using drag or paste operations, and the corresponding molecular formula and remaining structural field are created with a mouse click. Each entry also has an editable text field.

Switching back and forth between the three programs was surprisingly easy, but I frequently ran out of memory. ChemOffice requires at least 4 MB of RAM, System 7.0+, and (for color viewing) a color monitor. I evaluated this software using a Macintosh IIsi with 5 MB of RAM and System 7.0, but for most effective use of the program I would recommend more RAM, perhaps 8 MB. The memory shortage problem was averted, however, if all structures were saved frequently.

ChemFinder readily translates two- and three-dimensional structures between a variety of formats, as indicated in Table I. Thus ChemFinder provides a link to a variety of external software, including other computational chemistry programs and chemical databases. JMP statistical software of the SAS Institute Inc. of Cary, N.C., can initiate searches through the current version of ChemFinder. Version 2.0 of ChemFinder, due out this summer, will itself initiate searches of several external databases.

CSC CHEMDRAW PLUS AND CSC CHEM3D PLUS

The remaining two programs, ChemDraw Plus and Chem3D Plus, are quite impressive on their own merits and may also be purchased as stand-alone applications. They can be used individually or in concert in order to read and create chemical structures in a wide variety of formats (see Table I). The individual programs require only 1 MB of RAM and System 6.0.5+ and, for MM2 calculations, a floating point processor.

CSC CHEMDRAW PLUS 3.0.2

ChemDraw 3.0.2 continues the ChemDraw tradition of excellence in chemical structure drawing, and the new release has incorporated significant enhancements over the 2.*x* versions. One recent review rates ChemDraw 3.0 as "outstanding", a rating considerably higher than that given to ISIS Draw 1.01, and slightly higher than that for Chemintosh 2.1.[2] Even novices can master ChemDraw quickly, as the creation and manipulation of structures are analogous to other Macintosh drawing programs.

Particularly appealing in the new version of ChemDraw is that the two pointer options, lasso and marquee, can be accessed from a single tool. The text and atom label functions have also been combined as one tool, and the cursor is "smart enough" to know that an atom label is necessary when a bond junction is highlighted. In addition, selecting only one or a specified subset of atoms, bonds, text, or other features is much easier in ChemDraw 3.0 than in previous versions.

ChemDraw 3.0.2 comes with a large array of predrawn structures and substructures (>200!) that can viewed and edited, as well as additional tools for drawing arrows, orbitals, charges, and curves. ChemDraw 3.0.2 is System 7 savvy, supporting Publish and Subscribe, and Balloon Help, and supports Apple's AppleScript for performing user-defined sequences of commands. The program supplies a number of stationary pads that are preformatted for different publishing and presentation environments. The documentation claims that a ChemDraw picture can be edited directly from a Word 5.0 or WordPerfect 3.0 document, simply by double-clicking on the drawing, but the reviewer did not explore this feature. With ChemDraw Plus the pictures can be also be created, viewed, and printed in color. I found most of the new features very helpful and easy to use and needed to consult the documentation only twice; at those times I found the answers to my questions quickly. One feature I wish were available in ChemDraw Plus 3.0.2 is a multiple undo function.

CSC CHEM3D PLUS

Chem3D Plus 3.1.1 is equally impressive. To start with, any two-dimensional structure prepared as a ChemDraw document can be pasted into a Chem3D document and an appropriate three-dimensional structure is automatically created using standard bond lengths and angles! The three-dimensional structure can then be minimized, using a geometric optimization routine or, for Chem3D Plus, an MM2 energy minimization. Using the initial partially-optimized geometry, MM2 minimization of structures containing 10–20 heavy atoms did not take more than a few minutes using a Macintosh IIsi.

In order to evaluate the many features available, I completed the Tutorial in the Chem3D manual and quickly mastered the methods for creating, editing, and viewing structures.[3] In addition to conversion from ChemDraw and other chemical structure data formats (Table I), molecules can be created using substructures, bond tools, and an atom-type menu. Each structure is then rectified, automatically if desired. Molecules can be rotated using a track-ball-like feature, as well as rotation handles on the margin of the window. Multiple views can be created and run as a movie, and these can be exported to create a movie using Apple's QuickTime. In addition, a molecular dynamics calculation can be performed and easily translated into a movie.

Different atoms are represented by different patterns in black and white mode or, for Chem3D Plus, in color. These attributes can be easily modified as can a variety of other display options. For example, the model can be displayed in wire frame, ball and stick, cylindrical bond, or space filling modes.

The user can obtain information about atoms and groups of atoms in several ways. Pointing at or selecting one or more

Table I. File Translation Supported by CSC ChemOffice

	import formats	export formats
ChemDraw 3.0.2 Plus	ChemDraw (3.*x* and 2.*x*) connection table EPS MDL MOLFILE (Mac or text) MSI Mofile PICT SMD 4.*x*	ChemDraw (3.*x* and 2.*x*) connection table EGP (e.g. Word 5.0, Chem3D) EPS (Mac and text) MDL MOFILE (Mac or text) PICT SMD 4.*x*[a] SMILES
Chem3D 3.1.1 Plus	Alchemy Brookhaven Protein Data Bank Cartesian Coordinates Cartesian Coordinates with crystal cell parameters Cambridge Crystal Data Bank (FDAT) Internal Coordinates MacroModel MDL MOLFILE (Molecular Design Ltd.) MSI Mofile (Molecular Simulation Inc.) MOPAC files SMD 4.*x* SYBYL MOL (Tripos) SYBYL MOL2 (Tripos)	Alchemy Brookhaven Protein Data Bank Cartesian Coordinates connection table Internal Coordinates MacroModel MDL MOFILE (Molecular Design Ltd.) MSI Mofile (Molecular Simulation Inc.) MOPAC files ROSDAL (Beilstein) SMD 4.*x** SMILES SYBYL MOL (Tripos) SYBYL MOL2 (Tripos)
ChemFinder	ChemDraw 3.*x* or any format supported by Chem3D	ChemDraw 3.*x* or any format supported by Chem3D

[a] SMD, Standard Molecular Display, is the format used by STN Express for search Chemical Abstracts Online (CAS).

atoms results in the appearance of "Balloon-like" information panels containing values in any number of user-defined categories. Complete files for a single type of data for the compound (i.e. bond lengths) can be opened as a window, and if specific atoms are selected from the drawing, the corresponding values in the window are highlighted.

Energy minimization in Chem3D Plus is based on Allinger's MM2 parameters and force field.[4] CSC has added parameters for a wide variety of atoms and groups so that an optimization is seldom aborted due to missing parameters. One must use caution, however, as the new parameters are relatively untried, and the resulting geometries and energies may be inaccurate. On the other hand, Chem3D Plus has an editable parameter list that is easy to modify.

Chem3D Plus has been evaluated recently and compared to other microcomputer-based molecular modeling programs.[5] Chem3D Plus compared favorably with Alchemy II,[6] MacMimic,[7] and PCModel.[8] Chem3D Plus is among the best programs I have used, and some of its features, such as trackball rotation of a molecule, rival those of molecular modeling programs performed on workstations, which cost many times the price of a Macintosh II computer and Chem3D Plus. Other than the untested parameters for the MM2 implementation, the major inconvenience detected in Chem3D is that the large number of windows can be confusing if opened simultaneously.

ADDITIONAL COMMENTS

ChemOffice and its individual components would be an asset to many chemists. For the synthetic chemist, ChemFinder folders could be used to store compounds from the literature, as well as substrates and products for reactions performed. The text field in the database might contain relevant references or spectral data, and the two- and three-dimensional structures would be available for editing and pasting into a manuscript or proposal. The computational chemist will find the creation of MM2 optimized starting geometries very simple using Chem3D. Final geometries and energies could be stored in chemical folders using ChemFinder, facilitating organization of large amounts of output data.

ChemOffice was easy to install, and the documentation was adequate and indices comprehensive. While reviewing the package, I contacted Cambridge Scientific Computing by phone and through the Internet and received replies to my questions within 24 h.

CONCLUSIONS

The microcomputer-based modeling and drawing programs within ChemOffice are among the best available and are well linked through ChemFinder. ChemFinder folders are useful for storing and manipulating structural data, and the program has the potential for being a powerful interface with other applications and databases. A major complaint encountered in the past with CSC programs is the inability to share structural information with those in other computing environments. For ChemOffice, this difficulty remains, as versions of Chem3D and ChemFinder for other operating systems will not be available for some time. On the other hand, new versions of ChemDraw for Microsoft Windows and Unix will be released soon.

REFERENCES AND NOTES

(1) Cambridge Scientific Computing, Inc., 875 Massachusetts Ave., Suite 41, Cambridge, MA 02139.
(2) Jenkins, S. A. *MacSciTech* **1992** (Fall), 3–8.
(3) Chem3D 3.1.1 came with a Chem3D 3.0 manual and 3.1 supplement.
(4) Burkert, U.; Allinger, N. L. *Molecular Mechanics*; American Chemical Society: Washington, DC, 1982.
(5) Bays, J. P. *J. Chem. Educ.* **1992**, *69*, 209–215.
(6) Tripos Associates, Inc., 1699 South Hanley Rd., Suite 303, Saint Louis, MO 63144.
(7) Instar Software AB, Research Park IDEON, S-22370 Lund, Sweden.
(8) Serena Software, Box 3076, Bloomington IN 47402-3076.