TECHVIEW
SOFTWARE

Digital Chemical Intelligence

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In almost all fields of natural science—not just chemistry—sooner or later it becomes necessary to draw high-quality chemical structures and formulas. CambridgeSoft's ChemOffice is an all-in-one software suite that comprises not only the workhorse ChemDraw, but also a software program for creating and analyzing three-dimensional structures and modules, providing sophisticated search and information functions. CambridgeSoft offers its software in packages tailored to various tastes, needs, and budgets. The programs install from a single CD-ROM.

ChemOffice
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ChemOffice ULTRA, $1899 (academic discounts available).
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Undoubtedly, the cornerstone of ChemOffice is ChemDraw, a rigorous, independent drawing program that lets a user create structures of complicated chemical compounds in minutes. Novices to ChemDraw will be pleased to discover that the handbook is surprisingly well written and easy to understand. In six step-by-step tutorials, the beginner quickly learns to operate the most frequently used functions. The only drawback to the ChemDraw manual is that instructions for both Macintosh and Windows versions are combined in one text, often making it necessary to skim information for both systems.

ChemDraw is operated by a combination of tools and commands that can be selected from a tools palette and menu, respectively (Fig. 1). The tools palette includes drawing tools for a number of frequently used structural components, such as various common cyclic structures, and an Acyclic Chain tool. All of these tools deliver a structure with one click of the mouse. The Acyclic Chain tool allows the user to quickly draw carbon chains of variable length. Bonds can be drawn as wedges or lines, which can be solid, hashed, dashed, bold, or hollow. The Bond tool creates bonds that are fixed in their length and angle, but which can be changed as desired with a few mouse clicks.

The Orbital tool permits rapid drawing of s, p, d, and f orbitals. The Arrow tool offers a multitude of different arrows for reaction schemes, and the Pen tool delivers electron flow arrows. Charges, lone electron pairs, and radicals can be drawn with the Symbol tool.

The Text tool lets the user add atom labels, captions, and line formulas. For added convenience in ChemDraw, many of the keys on the keyboard have been preassigned to be "HotKeys." Each HotKey is reserved for the addition of an atom label or functional group to an existing structure so that the user need only point the mouse to an atom at the location of choice within a chemical structure and press the appropriate HotKey. ChemDraw automatically adds the proper number of hydrogen atoms to the label. The list of HotKeys that comes with the program is quite extensive but can be augmented and customized as desired by the user.

Another much appreciated feature is the Template tool (Fig. 2). With this tool, the user has access to a large number of templates that are stored in a folder accessible through the tool palette. It contains, among others, templates for amino acids, aromatics, stereocenters, polyhedrals, cycloalkanes, and hexoses, as well as DNA and RNA templates and 30 of the most common functional groups and bonds, such as ester and ether bonds, amino bonds, and carbonyl groups. These templates can be cut and pasted and are easily manipulated once they have been imported into the ChemDraw document. The template database can also be expanded by the user through new templates.

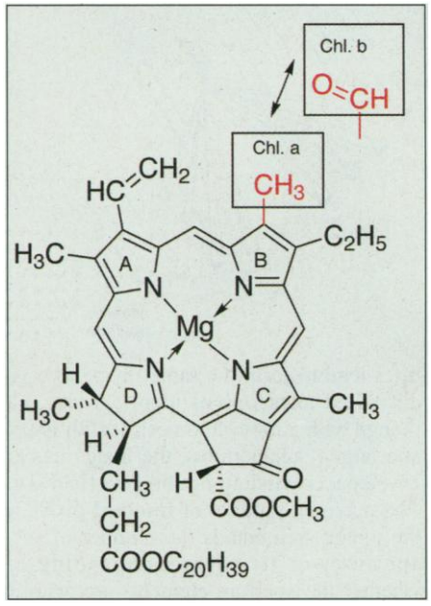

Fig. 1. A complex chemical structure, the light-capturing compound chlorophyll, as drawn with the ChemDraw module of ChemOffice.

Several file formats are available for exporting structures. Among the many options are the high-resolution tagged image file format (TIFF), which can be used for placing graphics into desktop-publishing applications, and the graphics interface format (GIF). GIF pictures are compatible with HTML files and, thus, are useful if structures are to be posted on World Wide Web pages. The handbook accompanying ChemDraw describes difficulties with picture exports to Microsoft Word through version 6.0. However, the program exhibited no problems exporting images to Microsoft Word 98 or PowerPoint 98 on the Macintosh.

To make it easy for the user to create camera-ready prints for publication, the settings for ChemDraw files can be saved on personal style sheets, which can be formatted according to a particular journal's specifications. ChemDraw also contains a number of preformatted style sheets with the settings required by some common chemical journals.

Another important feature that makes ChemDraw superior to standard drawing programs is its "chemical intelligence." Not only does ChemDraw automatically calculate the correct number of hydrogen atoms and add them to a given structure, but the program also has analytical functions: With the "check structure" function, any part of a structure or caption can be checked for chemical accuracy with an algorithm based on normal valences and elements, as well as a number of predefined "nicknames." These nicknames can represent substituents such as methyl, ethyl, or phenyl groups, but they can also represent a class of elements, such as all metals or all halides.

The "analyze structure" function calculates the molecular weight as well as the weight percent of each element and displays the molecular formula of a selected structure. The ChemOffice ULTRA version features an add-on function that provides the calculation of several physical and thermodynamic properties. These include (but are not limited to) melting and boiling point, critical temperature and pressure, and the Gibbs free energy. A "report" button lets the user view the references used for these calculations.

ChemOffice comes with a separate software program for molecular modeling and analysis, Chem3D. The Chem3D module is designed to assist scientists in modeling three-dimensional compounds. The software can be used for creating structures and for performing complex analyses of these structures. Of note are its molecular visualization capabilities. The user can

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choose to create a structure or to import structures from a large database of over 200 compounds.

Chem3D and ChemDraw structures are interconvertible, allowing one to conveniently sketch complex structures in ChemDraw for subsequent modeling in Chem3D. Using tools similar to those for the ChemDraw application, one can draw three-dimensional chemical structures in minutes. The molecules are automatically adjusted to display the proper number of hydrogen atoms. Users can choose to view the molecules as wire frames, stick models, ball-and-stick models, or space-filling models. Proteins may also be drawn as ribbon structures. Chem3D routinely draws all structures in trans conformation. These can, however, be easily converted into cis bonds. For three-dimensional viewing, molecules can be rotated about all three axes with the Trackball tool. This tool can reveal active sites in protein structures, areas of potential steric hindrances between or within molecules, helical portions of proteins, reaction sites, and so forth.

The analytical features of Chem3D range from simple computations of bond lengths and angles to analyses of complex properties such as steric energy, heat of formation, dipole moment, charge density, electrostatic potential, electron spin density, and atomic charges. The handbook supplied with Chem3D (hard copy and CD-ROM) explains the use of these analytical functions and provides useful background information about the individual properties. The methods used for calculating these chemical properties are also referenced in the manual.

Chem3D provides a graphical interface for the molecular computation application MOPAC (MOPAC is a trademark of Fujitsu Ltd., www.fujitsu.co.jp/index-e.html). A basic MOPAC application program is part of all Chem3D versions; however, only the professional version (Chem3D PRO) allows sophisticated calculations such as energy minimizations, transition state optimizations, and other advanced computations. A complete manual for the MOPAC application in Chem3D is included on the CD-ROM in Adobe portable document format (PDF).

With the professional version of Chem3D, molecular surfaces can be computed and displayed. Information about molecular surfaces of complex compounds is useful for predicting many chemical and physical properties. Extended Hückel surface calculations can be performed with Chem3D, providing information about solvent accessibility, total charge density, and organization of molecular orbitals.

Chem3D is also compatible with Gaussian, a program designed by Gaussian, Inc. (www.gaussian.com), for performing molecular orbital calculations. In contrast to MOPAC, Gaussian is not included in any version of Chem3D, but it can be purchased separately. When Gaussian (version 94 or later) is installed, Chem3D can provide a graphical interface for the application.

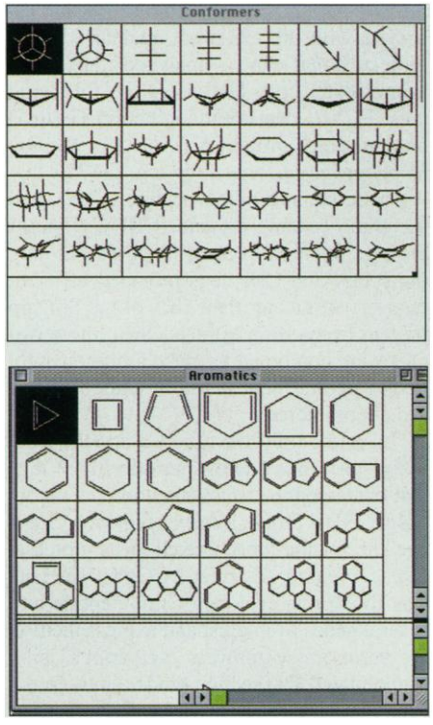

Fig. 2. Templates available in ChemDraw.

ChemOffice also is Web friendly. ChemFinder, the third member of CambridgeSoft's ChemOffice suite, indexes tables for searches and transforms ChemDraw files into tables. With databases such as MDL's Web-based Chemscape (Chemscape is a trademark of MDL Information Systems, Inc., www.mdli.com), the user can create customized chemical databases, import Structure Data (SD) files and MDL MolFiles, and convert them into tables using the MDL MACCS or ISIS/Base databases.

The Database Manager portion of ChemFinder provides an application for transforming tables into searchable databases on the desktop. With a few mouse clicks, queries can be performed and information is displayed in either their original tables or in new tables, which ChemFinder creates in seconds. ChemFinder is shipped with a manual that is divided in two sections: one for Macintosh users and one for Windows, relieving the user of the need to read versions for both Macintosh and Windows.

The fourth module of ChemOffice is ChemInfo. ChemInfo is a database in itself, containing chemical information. ChemInfo houses chemical names and structures, physical and safety data, and literature references. This wealth of information is only available, however, with the top-of-the-line Ultra version of ChemOffice. In addition, the database information is available on CD-ROM only for Windows users. In contrast, CambridgeSoft offers Macintosh users a year's worth of free access to their online database, a service which is normally available to anyone willing to pay an annual fee of roughly $50 to use CambridgeSoft's Chemfinder Web site (www.chemfinder.com). Nonregistered Web site visitors are granted free access to a portion of this chemical database that provides vendor information, links to vendors' online catalogs, and links to safety information Web pages, including the Occupational Safety and Health Administration's Web site. CambridgeSoft offers the potential customer a free, downloadable, demo version of ChemOffice 4.5 that is disabled in its "print" and "save" capabilities. This version is called the "Net version" and is an excellent way for the undecided customer or novice to ChemOffice products to determine which parts of the package offer applications that are most valuable to the individual user. The CambridgeSoft site also offers a number of free downloadable plug-ins, which enhance the usefulness of the software (http://store.camsoft.com/store/merchant.cfm).

ChemOffice offers technical support on the Web, by e-mail, or by telephone to registered customers. Although the employees were friendly and knowledgeable, the technical support line seemed to be understaffed—it took the author 5 days, two e-mails, and four phone calls to get a satisfactory answer regarding access by Macintosh users to the online ChemFinder database.

In summary, ChemOffice is a software suite that offers an outstanding array of chemical software. ChemDraw has been updated and revised enough times since its inception to eliminate many bugs from its earliest versions. It provides very user-friendly software for creating graphical representations of complex chemical structures in minutes. The companion program, Chem3D, delivers outstanding computing and modeling capabilities for research scientists and educators. Chem3D brings molecules to life and makes chemistry tangible for students in classrooms or researchers at the bench. The ChemFinder application is designed to help the user organize an ever-increasing flood of information in searchable tables and databases, and ChemInfo gives the researcher instant access to useful information.

ChemOffice includes versions for Macintosh and Windows. System requirements for Macintosh (OS 7.0 or later) and Windows 95 users include a minimum of 8 MB of RAM. Running the program with Windows NT 3.5 requires 12 MB of RAM.