# COMPUTER SOFTWARE REVIEWS

## ChemOffice Ultra 7.0

Robert E. Buntrock

Buntrock Associates, Inc., 11335 300th Avenue NW, Princeton, Minnesota 55371

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Starting in the mid 1980s, various information providers—including CAS and EI—began to realize that what technical researchers really needed was not just another source of information in their field, but that any kind of required data and information be available at their desktop. Not only should such a research workstation be able to access required information from a variety of sources, both internal and external, but also that the various inputs should be "massagable" into useful formats and reports. I assume the closest that one of the "traditional" A&I resources got was EI's Engineering Village, but that is still much more of a multifaceted Web resource than a "smart" workstation.

As a result, the chemist's workstation—and software to support it—was more logically forthcoming from various other software sources. ChemOffice Ultra 7.0 from CambridgeSoft is the latest in their line of tools for the chemist's workstation. I will not attempt to compare this package to others intended to accomplish the same or similar missions, but I will attempt to describe what this software package could do for the typical research chemist.

ChemOffice Ultra 7.0 for Windows (henceforth referred to in this review as "Ultra") allows the user with a desktop PC to manage various kinds of data and integrate the desktop with other systems, both external and internal to the organization. Ultra includes in the suite ChemDraw Ultra 7.0, ChemBats3D Ultra 7.0, ChemFinder Pro 7.0, E-Notebook Ultra 7.0, BioAssay Pro 7.0, interfaces for MOPAC, GAMESS, and Gaussian, ChemSAR Server Excel, CLogP, CombiChem/Excel, plus ChemInfo databases including ChemACX and the Merck Index (13th edition). Purchasing Ultra from ChemStore.Com on the CambridgeSoft Website (http://www.cambridgesoft.com)—at $2699—provides a 10% savings. For educators, the Website price of $1199 is a 60% saving. Discount pricing is also available for students, home users, and government employees. A free trial version is also available. For upgrade pricing, contact CambridgeSoft. For users not part of an organizational Intranet, versions for individuals are also available.

Additional description of ChemOffice Ultra 7.0 can be found on a related Webpage (http://products.cambridgesoft/com/ProdInfo.cfm?pid=234). Features new to this version include Polymer Draw (polymers in ChemDraw), BioArt (biochemistry symbols), ChemDraw/Excel 7.0, Online Menu 7.0 (vendor information from ChemACX.Com), Purchasing for Excel, ChemSAR Server/Excel (calculations performed in ChemBats3D), atom numbering (sequential numbering of atoms in structures), and MS Word numbering (assignment of reference numbers to ChemDraw structures in MS Word documents).

Ultra contains two drawing tools: ChemDraw Ultra 7.0 and ChemBats3D Ultra 7.0. Reviewing all of the capabilities of these tools would require a separate monograph for each. Suffice it to say that both packages are very powerful and have a wide variety of uses. As part of ChemDraw, ChemNMR can be used to predict $^{1}H$ and $^{13}C$ NMR line spectra. IUPAC names can be generated from structures and structures can be generated from many names. ChemProp can be used to calculate physical properties from structures. Structures can be drawn within the program or imported from other sources in a variety of formats including SMILES strings. Structures can be exported to a variety of other documents and files.

Structures can be drawn in ChemBats3D or imported, either from ChemDraw or ISIS Draw. Structures and models can be manipulated or displayed in a wide variety of ways. Even more powerful calculations of properties or transition state geometries are available, using ChemSAR for Excel or MOPAC Pro. The latter includes AM1, PM3, MNDO, MINDO/3, and MNDO/d. Visualizing MOPAC results with surface property mapping is featured. Gaussian calculations are available through a client interface, and GAMESS computations can be performed by downloading the GAMESS application separately.

I intend to use ChemBats3D to further explore an abandoned project from my thesis days. Hopefully I can establish to my own satisfaction that 4.4.4-propellane is chiral and possibly even capable of resolution into conformers.

E-Notebook can be used to either enhance the capabilities of a laboratory notebook or even replace it. It is either a standalone application or it can be used with other programs, including Microsoft Word and Excel, or can be used to interact with other users in your organization via an Intranet. For organic syntheses, storable information includes stoichiometric calculations (automated), reaction and preparations, analytical methods, notes, and spreadsheets. E-Notebook can be searched by structure and substructure or reaction transformation.

Ultra ChemOffice also includes a document manager for performing administrative functions for documents throughout your organization. Associated search logic includes left and right truncation and an extensive list of text searching operators including the usual Boolean operators plus more advanced functions including "fuzzy".

Databases are also included in the package. ChemINDEX has small molecule data from the Web and NCI. Included is BuckyBase, a file of 132 fullerene/Buckyball molecules. The NCI file includes 246 620 compounds tested by NCI with test data. AIDS test data is included if present.

ChemMSDX contains over 7000 material safety data sheets for common lab chemicals.

ChemRXN includes ChemSelect, a file of ca. 13 000 reactions from InfoChem Gmbh, and ChemPrep, a sample of ca. 25 000 chemical reactions from ISI ChemPrep. Both files are searchable by structure and data elements and both contain related subfiles on catalysts and solvents, separately searchable and displayable.

A ChemOffice version of The Merck Index 13th Electronic Edition is also included. This is the latest edition of this desktop "bible" and contains >10 000 monographs of compounds and groups of compounds. It is searchable by structure, substructure, names, activity categories, and data elements.

However, unlike my standalone version of the 12th edition on CD, the "browse" mode of searching has been deactivated in this version. This is unfortunate because the use of browse in a database of this size facilitates finding pharmaceuticals known only to the user by name and often with uncertain spelling. Name searching with both left- and right-hand truncation would also be useful.

Databases new to ChemOffice Ultra 7.0 include ChemACX 7.0 (access to 300 catalogs of chemical suppliers of >450 000 compounds) and ChemACX-SC 7.0 (searchable catalogs from screening compound suppliers).

I will leave it to the prospective purchasers to make comparisons to other software packages dedicated to the same purposes. However, I hope that I have given enough of a synopsis to pique your curiosity about testing ChemOffice Ultra 7.0 for yourself and for your organization.

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