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COMPUTER SOFTWARE REVIEWS

ChemDraw Ultra 10.0. CambridgeSoft, 100 CambridgePark Drive, Cambridge, MA 02140. www.cambridgesoft.com. Commercial Price: $1910 for download, $2150 for CD-ROM; Academic Price: $710 for download, $800 for CD-ROM.

ChemDraw is the "industry standard" chemical drawing package, as evidenced by the fact that ACS journals refer to ChemDraw in the instructions to authors for the preparation of chemical figures. Newer versions of ChemDraw are more than just drawing packages; rather, they are analytical tools, allowing the calculation of exact molecular weight, elemental analysis, *m*/*e* for the parent ion, including isotopic abundances, proton and carbon chemical shifts, boiling/melting points, critical pressure and temperature, and ΔH_f. The newest version, ChemDraw Ultra 10.0, includes a subroutine that will calculate the stoichiometric quantities for a reaction (see below for more details). This version is also integrated with Chem3D, allowing three-dimensional visualization of molecules, E-Notebook for electronic record-keeping, Mestrec-Lite for processing of NMR data, and ChemFinder.com to locate physical properties of molecules. ChemDraw offers "one-stop shopping" for molecular information, in addition to providing a convenient way to create professional molecular drawings.

ChemDraw Ultra 10.0 has several features that are either new or improvements on existing versions of the program. One feature that is particularly useful is the stoichiometry grid. With it, you simply draw the reaction, select as a group all of the reactants and products, and choose "analyze stoichiometry". A grid appears in which you can identify the limiting reagent and the amount of that reagent, and the program will calculate all of the other amounts needed and the amount of product formed. If you are using a solution, you can enter the molarity and volume. When the product is isolated, that information can be included to get percent yield. This is not a crucial feature, but I can see that it has the potential to make life simpler. In addition, there are some smaller changes that remove some previous irritations. In older versions of ChemDraw, you could select an object and rotate or resize it; in the newest version, you can also resize in one dimension, that is, make the structure "fatter" or "taller". Rectangles and ovals can also be adjusted in one direction, giving a fat or skinny oval. The arrows tool has more types of arrows and, more importantly, allows the angles of the arrows to be modified.

Other improvements to ChemDraw Ultra 10.0 from 7.0, my previous version, include "disequilibrium" arrows that indicate in which direction the equilibrium lies and double-headed arrows. There are more chemical symbols, including a greater variety of "attachment" points, allowing the structure to be attached to a bead, for example. Version 10 has a template for a TLC slide that can be modified for different numbers, types, and shapes of spots. There are more predrawn templates, including a variety of nanotubes, polypeptides, supramolecules such as calixarenes, and amino acid side chains as well as the amino acids themselves. The BioArt structures are augmented by additional structures, e.g., immunoglobulins, endoplasmic reticulum, etc., and a periodic table can be easily accessed. Finally, the fragmentation tools allow you to evaluate the mass of the fragment of a molecule easily. The documentation is good, and the tutorials are excellent. Much of ChemDraw is intuitive, so the learning curve for a new user is not steep.

With regard to the integrated modules, Chem3D Standard allows visualization in three dimensions and as a variety of types, including as a space-filling model that can be incorporated into a ChemDraw document. It also does molecular mechanics calculations and provides an input to common computational packages, such as GAMESS and Gaussian. E-Notebook is designed to replace the hand-written lab notebook, with enhanced organizational capabilities. The NMR processing program, Mestrec, is an excellent addition to the suite of programs. It was originally distributed as a free program from a group of chemists in Spain, but current versions are only available for a fee. The Lite version included in the suite will only process 1D data sets but can handle data from any type of FT-NMR spectrometer. Our students prefer processing their data with Mestrec rather than using VNMR from Varian, so it is a very user-friendly program. The cost of an individual license of Mestrec-Lite is $128 at the current conversion rate from Euros, so this can be considered part of the cost of ChemDraw Ultra.

There is a great deal of functionality in the ChemDraw Ultra suite. It is, however, pricy, and the question becomes whether the functionality is worth the price, both for users who already have a copy of ChemDraw and are thinking of upgrading and for those who are using a minimally functional drawing program and are thinking of moving to ChemDraw. The analytical tools listed in the first paragraph are nice but must be used with some caution. The calculation of molecular weight and isotopic abundances are reliable, but the calculated NMR shifts are useful only as a guide. Similar comments apply to the calculation of boiling/melting points, critical pressure and temperatures, and heats of formation. I spoke with one of our biochemists about the BioDraw tools, and she felt that they were nice but not essential.

What are the alternatives to Chem Draw Ultra 10.0 for a person who needs to upgrade, who has lost access to ChemDraw because of a change of job or location, or who has never had access to ChemDraw? ISIS-Draw has a free chemical drawing program with limited functionality. It is very satisfactory for the price but would be aggravating to chemists who need to draw a number of structures. The templates are limited in scope, as is most of the functionality. It is simply a bare-bones drawing program. An alternative would be to purchase an older, more limited version of ChemDraw. Cambridgesoft offers a download version of ChemDraw Ltd 9.0 for $380, commercial; $70, academic. It has many of the features attractive to chemists, including the trackball to modify the perspective of a structure,

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a substantial number of templates, and limited analysis of chemical properties, which does not include the calculation of NMR shifts or thermodynamic properties. It also does not offer the additional modules: Chem3D, E-Notebook, and Mestrec.

Who should buy ChemDraw Ultra 10.0? The features available in this version have the potential to really save time when constructing graphics of publication quality. Also, the analytical tools including Mestrec Lite offer the promise of greater efficiency in the planning, implementation, and analysis of experiments. In industrial and graduate school environments, the electronic notebook is probably very appropriate. For undergraduates, graduate students, and faculty with more limited needs for preparing chemical structures, ChemDraw Ltd 9.0 is more appropriate on a cost/benefit consideration. Would I purchase ChemDraw Ultra 10.0? I would seriously consider it if I had an unexpected pot of grant money. It is a really nice program with a lot of functionality. However, as is true with many bundled programs, there is more functionality in the program than is absolutely crucial for most users.

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