

COMPUTER SOFTWARE REVIEWS

Chemistry 4D-Draw Version 2.0 for the Macintosh or PC with Windows

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Chemistry 4D-Draw¹ is a new version of this program which replaced **ChemNamStru** in March 1995. The Windows version was tested, but it is assumed that the Macintosh version is directly comparable.

The program was installed and used under both Windows 3.11 and Windows 95 (Prerelease Version). Installation was quite straightforward and resulted in a Chem 4D-Draw icon (a very clever icon based on a benzene ring but spelling ChemInnovation) which, on double clicking, started the program. Program control is via a vertical tool bar containing an array of 30 icons, a horizontal Windows-type drop down menu bar of nine parent items and a horizontal "speed-bar" of 11 icons (new document, open, save, duplicate, cut, copy to clipboard, load from clipboard, undo (seven levels available), reverse-undo, print, and print page to screen). Some of these differed from the normal Microsoft icons but were clearly self-explanatory. The program was very easy to use, most operations being completely intuitive, hence a "point-and-click" user will have no problem getting rapid results. For assistance the on-line Help is excellent and well structured, and the 58-page manual is full, clear, and well structured. In particular it contains six tutorials to introduce the user to all main aspects of the package.

Chemistry 4D-Draw is directly comparable to other major chemistry drawing packages which are considerably more expensive. It lacks options to import and export structures which use other storage formats (e.g., Molfile format), but it has many compensating advantages. Features which I particularly liked include the following: molecules or fragments can be rotated in three dimensions, sequence numbering can be displayed and modified, it is intelligent in accepting only existing elemental symbols, and, while it checks valence numbers and reports inconsistencies, it does allow the display of incorrect valence when in radicals, etc. Structures can be exported using OLE-2 technology so that it is simplicity itself to incorporate them in, e.g., MS-Word documents. The program handles superscripts and subscripts smoothly and supports multiple documents allowing the user to work in a number of documents simultaneously and compare the results on screen at the same time.

A feature in Chemistry 4D-Draw which is absent in other comparable packages is the **NameExpert** module. This

allows the user to type in a IUPAC approved name (or many trivial names), and the structure is displayed in a variety of formats. This is a splendid feature, particularly for students and teachers, and alone would justify buying the program. Chemical nomenclature is alarmingly complex and not necessarily logical to computers so that problems are to be anticipated. In general, the program handles correct IUPAC names very well and is excellent for teaching purposes. Some groups are not yet included, but these can be accommodated by using more complete variants, e.g., in place of oxime use *N*-hydroxyimino. The manual demonstrates some of the wide range of complicated structures which can be named. Many trivial names are recognized, and the program is surprisingly forgiving to omitted hyphens and other minor errors. If sequence numbers are omitted it generally makes an intelligent "guess", but this can lead to problems so structures using trivial names must be checked carefully. For example, entering *oxazole* gives the structure for furan, while *1,3-oxazole* and *2-aza-5-oxa-1,3-cyclopenta-1,3-diene* give the correct structure. Isoxazole, on the other hand, gives the expected structure. Unfortunately it does not recognize phosphonic or phosphinic acids, and it interprets phosphines and arsines as analogues of pyridine rather than ammonia. However these are comparatively minor problems compared to the overall power of the module and its usefulness to both students and teachers.

Chemistry 4D-Draw can be recommended enthusiastically. It is both very powerful and easy to use and is also very reasonably priced, especially for academic and student users. It is ideal for preparing manuscripts and reports, and any chemistry department which takes out a license to use it for teaching will find it an invaluable teaching aid.

REFERENCES AND NOTES

- (1) Chemistry 4D-Draw is produced by ChemInnovation Software, 8190E Mira Mesa Blvd., No. 108, San Diego, CA 92126, U.S.A. Phone: 619-566-2846; Fax: 619 566-4138. The price is \$199 with generous academic and student discounts.

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