before they are inserted into the various documents, as well as for adding lines, boxes, arrows, etc. to the images using a variety of pen styles and widths. Text in 12 different fonts can be added anywhere on the screen. Complex chemical and mathematical formulas and equations can easily be created by using the Main editor.

The Document editor is a powerful word-processing program that contains a few additional features rarely found in most word processers such as editable macro commands and windows for viewing up to nine documents, any two of which can be seen on the screen at the same time. Boldface, italics, underline, and/or any combination of these, superscripts, and subscripts, as well as nine different fonts or typeset (e.g., Greek, Fraktur, Cyrillic, script, mathematical symbols) can be used with this editor.

The Molecular editor is used to create new molecules or to edit existing ones. Molecules are created by freehand drawing or by using predetermined templets (58 of those are available). One may also save his/her own templets (their number is practically unlimited). Once created or edited, the molecule could be saved as a molfile or placed anywhere in a document. As a matter of fact, this editor is identical with the one in CHEMBASE, which is another component of MDL CPSS.

The Reaction editor is used to create new reactions or edit old ones. Once created or edited, the reaction could be saved as a rxnfile or placed in a document. This editor is identical with the one in CHEMBASE.

The Form editor is used to create new forms for displaying structures and data or to edit old ones. Once created or edited, the form could be saved as a file or placed in a document. Like the other editors, this one is also identical with the one in CHEMBASE.

The program consists of nine disks (eight disks and a backup of the program disk) and a user guide in two parts (the first part, 196 pp, contains installation instruction and a tutorial; the second part, 240 pp, deals with the various components of the program). The manual is very clear and easy to read and use. Besides the manual, the program comes with a very good Quick Guide as well as a Quick Reference that lists and explains the various program commands.

The program seems to be so interesting and the Quick Guide is written in such a way that one tends to try to explore it even before reading the manual, usually with considerable success.

The program includes some tutorial files that could be edited into a whole document containing text, sketches, molecules, etc. The tutorial manual tells the user step by step how to use the program in order to create and print a finished complex document—an excellent idea that makes one immediately familiar with the program even before learning all its commands. Another interesting feature are the detail help screens available anywhere along the program. These help screens are of two versions: one version for the novice user, another for the expert.

All the commands in the Molecular, Reaction, and Form editors as well as those of the main menu are chosen from pull-down menus. The situation is somewhat different in the Document editor, where they are all keyboard commands; however, most but not all are also menu chosen.

Text and images can be imported to CHEMTEXT from other Molecular Design Programs: CHEMBASE, MACCS, MACCS-II, REACCS, and CHEMLAB-II. The program contains some tools for the conversion of RS/1 files and HP-GL plot files into MDL format metafiles, thus enabling their incorporation into CHEMTEXT.

One really cannot see on the screen how the printed page would look. To see it, one has to use the print preview function (e.g., right-hand justification is not shown on the screen; however, it is seen in the page preview).

There is one main feature that is missing in the program, and I hope it would be included in a later version—the undo command. Although in the Form editor there is an undo command that throws away any changes that were made in the form since one entered the editor, it does not restore a structure that was cleared with the Clear Structure command. Indeed, one may cancel a command, but it works only before the command is executed. However, if cancellation is given during execution, whatever had been carried out could not be returned to the "original" situation.

Another problem that limits to some extent the usefulness of CHEMTEXT is that files cannot be transferred to mainframes for storage or printing (when one has a laser printer under a Vax or a Prime) unless CHEMTALK is used, or that dot-matrix or postscript files are used. The problem with these files is their size. A 10-page document is about 400–450 kB—a huge file to transfer or save (although it can be done).

To sum up, we have here a very good chemical word processer, which has been needed for a long time. This program enables the chemist as well as the scientific secretary to compose and print a document containing complex chemical and/or mathematical formulas in a short time and with good quality. The only inhibitory factor for purchasing this package is its price, which is $1500. For universities there is a reduced price of $500. In keeping with the recent enlightened attitude of software companies toward their users, the program is not copy protected.

ChemIntosh and ChemPanion, Organic Structure-Drawing Desk Accessories for the Apple Macintosh†

ALLAN L. SMITH
Chemistry Department, Drexel University, Philadelphia, Pennsylvania 19104

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As chemists began during the past 15 years to prepare manuscripts for publication using computers, the first software to become widely used was word processing. Word processors initially had line- or string-oriented user interfaces, since their progenitors were line-oriented text editors. But much of the chemical literature uses embedded chemical structure drawings that could not be handled with a character-based screen editor. With the advent of bitmapped displays such as the Apple Macintosh, however, screens could be painted pixel by pixel, and the potential existed to produce on a personal computer chemical manuscripts that intermingled text and graphics.

Since the Macintosh has a standard method (the clipboard) of transferring data from one software package or "application" to another, the first approach taken by chemists using Ma-

† Version of software reviewed: 1.2 (both ChemPanion and ChemIntosh). Publisher: Softshell Co., 88 Fox Chapel Road, Henrietta, NY 14467. Hardware requirements: Macintosh 512KE, Macintosh Plus, Macintosh SE, Macintosh II.

cintoshes was to draw chemical structures with existing graphics programs such as MacPaint or MacDraw. Transfer of these structures to word processors such as Microsoft Word or Apple's MacWrite was effected through the clipboard. The next major advance in organic structure drawing for the Macintosh was the software package ChemDraw,[1] by Cambridge Scientific Computing. ChemDraw has a palette of graphics tools specific to organic structure drawing and many additional features and tools designed to simplify the task of creating complex molecular figures. To merge MacPaint, MacDraw, or ChemDraw structures within the text of a manuscript, one must copy to the clipboard, quit the application, open the word processor, and then paste. Another method employs Apple's Switcher utility, set up with the drawing program in one window and the word processor in the other.

There is a class of programs for the Macintosh, however, that act very much like memory-resident programs in the IBM PC in that they can be used while another program is still active in memory. On the Macintosh this type of program is called a desk accessory. ChemIntosh and ChemPanion are Macintosh desk accessories for drawing organic structures. ChemIntosh, the more expensive of the two, has all of the features of ChemPanion and several others (see below).

As Macintosh desk accessories go, ChemIntosh and ChemPanion are quite large. The ChemIntosh desk accessory and a required additional resource take up about 330 kB of disk space; ChemPanion's corresponding size is about 280 kB. The use of ChemIntosh and ChemPanion on Macintosh 128K or 512K systems with 400-kB disk drives is thus problematical, although telephone support from the publisher is quite helpful in pointing out ways to work around these limitations. I tested both programs on a Macintosh 512KE with one 800-kB drive and found that with ChemIntosh there was about 100 kB of available space on a disk with a good-sized system file, the Finder, the Imagewriter Driver, and MacWrite. On a Macintosh Plus, SE, or II these space problems disappear, especially with a hard disk.

The ChemIntosh and ChemPanion user interface has a palette of 22 icons representing both structure fragments and tools; another 22 can be displayed by depressing the CapsLock key. Getting used to this interface takes a little more time than for a normal Macintosh application because of the absence of pull-down menus. Chemical string symbols are entered in a one-line panel at the top of the screen. Dialogue boxes with concise, in some cases even terse, help messages can also be invoked through a question mark icon. There are many graphic tools in ChemIntosh and ChemPanion for creating chemical structure diagrams: rings with from three to eight carbons, including benzene, chair and boat cyclohexane, and two cyclopentanes; a variety of bonds (wedged, hatched, wavy, dashed, as well as standard single, double, and triple bonds); arrows depicting reaction, equilibrium, resonance, and electron movement in reaction mechanisms; special symbols such as brackets for repeating groups and a stereochemistry dot.

The primary difference between ChemIntosh and ChemPanion is that in the latter structures cannot be saved to files or read in from files, nor can they be printed directly from the desk accessory, whereas in the former they can. Since desk accessories are by definition meant to be used with other programs, the lack of file input/output and printing for ChemPanion is not really a serious limitation because the parent application always has these capabilities. It is even possible (see below) to create databases of structures in a word processor or file manager by using ChemPanion.

The manuals for both ChemIntosh and ChemPanion are written in exceptionally clear and economical prose and are thoughtfully organized. After an introduction, a Quick Start section "for the Experienced Macintosh User" summarizes the capabilities of the software. Following this is a "Tutorial—for the Newcomer", a longer section for first-time Macintosh users who need some of the jargon explained (e.g., the difference between close, zoom, and grow boxes). There is a short Reference section describing each icon, its associated operations (click or drag), the result, and options. Both the Glossary and the Index are complete and easy to read. The manuals themselves are fine examples of how ChemIntosh structures can be smoothly merged into the flow of text.

As a test of ChemIntosh, I turned to Schaum's Outline Series volume, *Theory and Problems of Organic Chemistry*,[2] and attempted to duplicate on the Macintosh screen all that I saw on a portion of a page. I was, for example, able to reproduce exactly the structure drawing illustrating the following sentence: "Hydration of the middle carboxyl group in ninhydrin removes both pairs of repulsions". Greek text symbols indicating partial charges were easily generated (with the standard Geneva font) and accurately placed around the structure. I tried several other pages, with excellent success. The only problems I had were trying to draw long and nonsymmetric curved arrows in reaction mechanisms and in generating a pair of Lewis dots (the former problem can be overcome by copying the figure to MacDraw and editing further, and a symbol for the Lewis dot pair can be created as a special character in a font with Apple's Resource Editor). With MacWrite, ChemIntosh structures (and indeed any other graphics pasted into text) occupy full lines, so that it is impossible to flow text smoothly around small organic structures in-line. With other more powerful word processors, however, this limitation does not apply.

Of particular interest is the capability of both ChemIntosh and ChemPanion to accept structures created earlier and pasted into word-processing documents, again through the clipboard. This permits the user to create whole families of related structures easily by minor editing of previous structures embedded directly in the text of a paper. As a further test of this capability to use figures previously created, I used ChemIntosh with Filemaker Plus,[3] a database management program. Using the fact that fields in Filemaker Plus can be of form text, number, or picture, with an hour's work I built a database of half a dozen structures, with each record containing the chemical name, the molecular formula, and a structure diagram. While I encountered a few memory problems in the process, I could usually circumvent them. This exercise convinced me that the idea of a structure-drawing desk accessory has considerable potential for the chemist with a Macintosh.

ChemIntosh costs $295 and ChemPanion costs $149, with 20% academic and 60% student discounts. While I have not attempted a comparative review of ChemIntosh and ChemDraw here, several of my colleagues who use ChemDraw and who watched me demonstrate ChemIntosh remarked that there are features in ChemIntosh not available in ChemDraw. You can get a demonstration version of ChemIntosh directly from SoftShell Co. in order to explore this point further. As an infrequent drawer of organic structures (I am a physical chemist), ChemIntosh certainly appears to be able to meet all of my needs, and I recommend it highly.

REFERENCES AND NOTES

(1) ChemDraw, V 2.0, Cambridge Scientific Computing, P.O. Box 2123, Cambridge, MA 02238 (617-491-6862).
(2) Meislich, Herbert; Nechamkin, Howard; Sharefkin, Jacob. *Theory and Problems of Organic Chemistry*; Schaum's Outline Series in Science; McGraw-Hill: New York, 1977.
(3) FileMaker Plus, Nashoba Systems, Inc., 175 Sudbury Rd., Concord, MA 01742.