# Computer Software Reviews

**ChemText. Version 1.10.** Molecular Design Limited: 2132 Farallon Drive, San Leandro, CA 94577. List Price $1500 ($500.00 Academic).

ChemText is one of three components of Molecular Design Limited's (MDL) Chemist's Personal Software Series (CPSS). ChemText is a word processor designed specifically for chemical applications that can integrate structures, forms, and equations into the text of a document. It can also be used to create sketches and drawings suitable for slides or journal illustrations. The other two components of CPSS are ChemBase and ChemTalk. ChemBase, a molecule and reaction data base manager with sophisticated search and visual display capabilities has been reviewed in *J. Am. Chem. Soc.* **1987**, *109*, 2230. ChemTalk, a communication program that can link a PC to a host computer running MACSS-II and REACCS, has not been examined by this reviewer.

ChemText is designed to run on an IBM personal computer (PC, PC XT, or PC AT and 100% compatibles). A minimum of 640 KB memory, a graphics card (Hercules, IBM color graphics adapter or IBM enhanced graphics adapter with 128 KB graphics memory), and a mouse (Mouse Systems serial or Microsoft bus or serial mouse) are required. A Hard disk with a minimum of 10 MB is required; the files necessary to run ChemText occupy roughly 1.5 MB. Printer support is discussed in detail below.

ChemText is not copy protected, and ChemBase is now available without copy protection. It is licensed for use on one computer by one user at a time. ChemText comes on 9 floppy disks—a system disk, three font disks, two support disks, a utilities disk, and a program disk (2 copies). Backup copies can be made. Chemtext 1.1 is compatible with version 1.1 of ChemTalk and ChemBase, but not fully compatible with earlier versions of these programs.

ChemText is both a word processor and a structure and equation drawing program. Unlike most chemical drawing programs, structural information is stored in a chemically meaningful manner. This has some advantages within ChemText since hydrogens on heteroatoms or terminal carbons can be added automatically and Chemtext will tell you if a valence is exceeded. However, the main advantage of this mode of data storage is that it allows files to be exported to, or imported from, ChemBase on the PC or from MACCS-II and REACCS on a main frame computer.

There are five separate editors. The document editor is a word processor. The molecule editor is used for drawing molecules. The main editor is used to combine molecules and reactions into complex sketches and to create complex equations. The reaction and forms editor are used primarily to create files for use with other MDL programs.

The document editor is a powerful word processor specifically designed for chemical applications. The word processor functions in either a menu or command driven mode. Unlike many word processors on the IBM PC, extensive use is made of popup menus selected by a mouse. This makes this word processor very easy to learn and operate for inexperienced users. For those more advanced, these commands are also accessible by holding down the CTRL key and entering a one- or two-letter acronym code. A few commands are not accessible from the mouse menu and must be entered with a CTRL code.

Two cursors are displayed; the text cursor functions as in other word processors while the mouse cursor is displayed as an arrow about $^1/_4$ of an inch long. The mouse cursor is used to select commands from the menu and, if desired, to move the text cursor by large increments and define blocks of text.

Characters are displayed on the screen in graphic mode so that superscripts, subscripts, boldface, italics, and underline are seen as they will appear when printed. Numerous fonts are available including undersized, European characters, Cyrillic, Fraktur, Greek, Script, and two sets of Math Symbols. When an alternate font is selected a font table for keyboard conversion is displayed on the bottom of the screen. All fonts also appear accurately on the screen. Subscripts and superscripts are accessed easily by using shift ↓ and shift ↑. These are displayed on the screen shifted vertically in the undersized font. With the Hercules graphic card available to the reviewers, both documents and structures are attractively displayed on the screen.

The document editor contains most features found in word processors. Margins and tab settings are displayed on the bottom of the screen and can easily be modified. If modified they apply to that paragraph and any following paragraphs until they are again reset. Headers and footers can be inserted in many styles. Blocks of text can be selected and moved, deleted, inserted, copied, appended, and printed. Text strings can be searched for (with or without replace). Macros can be constructed and used to simplify repetitive procedures. Mail merge capabilities are not available automatically but can be constructed by the user using macros. Windows for viewing up to 9 documents are available. Two documents can be on the screen at once. The document editor does not have a spelling checker or a thesaurus, although these are planned.

The following printers are supported: Epson FX, MX, RX, FX+; Okidata 92, 93 with Plug 'N Play; IBM Proprinter, Toshiba P351, P1340, P1350, P1351; Hewlett-Packard ThinkJet; Hewlett Packard LaserJet Plus and LaserJet Series II preferably with either the D, G, J, or M elite font cartridges; Apple LaserWriter. "Presentation quality" documents are produced on the Apple LaserWriter. The output on the Hewlett-Packard LaserJet Plus or LaserJet Series II is printed at full resolution, 300 dots per inch (dpi), *only* for text with the standard font. All other fonts and chemical structures are printed at 150 dpi which produces output which is clearly not "presentation quality". ChemText does not make use of the available compressed, greek, and math symbol fonts on the J cartridge but instead creates its own noticeably poorer characters in a 150 dpi mode. Documents containing subscripts or superscripts cannot be printed single spaced except on the Apple LaserWriter. The printer drivers cannot be modified by the user.

Prior to printing, either 10 or 12 pitch can be selected. Documents are reformatted during printing. Three print modes are available: (1) immediate which halts all other functions till printing is complete, (2) background which allows editing to continue, and (3) printing to disk which creates a file that can be printed at a later time with only DOS commands. This allows files to be printed from computers on which ChemText is not installed. However, files produced in this manner that contain structures or alternate fonts are very long; a page can easily be 100 KB. Normal text and structure files that can only be read and printed by Chemtext are comparable in length to those created by other word processors and drawing programs on the IBM PC.

Molecules are drawn in the molecule editor. Structure drawing can be accomplished very rapidly with the mouse. A "Clean" command converts initial freehand mouse input into regular polygons or chains. Bonds, atoms, and fragments can also be moved and adjusted and resized. Templates are available, including 14 rings, 11 polycyclics, 14 chains, and 19 functional groups; others can be easily added. Templates can be attached by connecting an atom to a point on the structure or by fusing a bond to a bond on the structure. Bonds are always drawn as single bonds initially, but they can be changed to double or triple bonds or wedges, hatches, or jagged stereo bonds. Any atom can be specified in a label, and its valence, charge, or isotope number can be specified with simple commands. Hydrogens on terminal carbons and heteroatoms can be added and removed automatically by selecting the appropriate mode.

Sketches are created in the main editor by combining molecules created in the molecule editor and adding lines, straight and curved arrows, boxes, and text as desired. Images may need to be resized to fit on a sheet of paper. Text used as atom labels in molecules is a standard size which is not resized with the rest of the structure but can be resized in a separate operation. However, text inserted in the main editor can use all of the fonts described above plus 24-pt Roman and 6-, 8-, 10-, 12-, 18-, 36-, or 48-pt Helvetica. Sketches and molecules are shown on the screen as they will appear when printed.

Sketches can be printed by themselves or inserted into documents. When a sketch is inserted into a document an "anchor" is shown which allows the image to be moved, deleted, or searched for as if it were a single character. The sketch is shown in the appropriate place in the document.

Construction of structures in a chemically meaningful manner, so that they can be transferred to and from a database, has obvious advantages, especially for those who are users of other MDL programs. However, for those who are interested in using ChemText as a drawing program this approach is somewhat cumbersome since molecules must be drawn in one editor and then stored as a molecule file. Molecules must then be combined in a second editor to make a finished structure.

Simple equations can be constructed in the document editor. Complex equations are best constructed in the main editor as a series of short text strings which can be in different fonts. The text strings are placed on the screen and moved together to give a complete equation which is inserted into the document as a sketch. If the equation appears correctly on the screen, it will print properly.

ChemText is complex, as one would expect for such a sophisticated

program. A very complete, two-volume, ≈500-page manual and 40-page "quick guide" are provided. The system also includes more than 400 screens of online help for novices and 80 screens of more compressed information for experts. Sample document, molecule, and image files are provided along with an easy to follow and well-designed "tutorial" which takes about an hour to complete and covers constructing molecules, sketches, and documents and combining molecules into sketches and inserting images into documents. Installation can be accomplished easily and almost automatically by following instructions on a setup menu.

In combination with an Apple Laserwriter, ChemText provides an attractive method to prepare "presentation" quality documents containing structures and equations on an IBM PC. It is an excellent scientific word processor but does lack some of the features found in dedicated general purpose word processors.

**Barry Snider,** *Brandeis University*

# *Book Reviews* *

**High-Performance Liquid Chromatography. Advances and Perspectives. Volume 4.** Edited by C. Horvath (Yale University). Academic Press: New York. 1986. xi + 321 pp. $70.00. ISBN 0-12-312204-X

This volume is the fourth in a series of books that deal exclusively with HPLC. The editor's goal is to provide up-to-date accounts of new developments in various areas of HPLC. To this end he has been very successful in enticing well-known chromatographers to write authoritative reviews on topics ranging from instrumentation to applications. As with the previous 3 volumes, the quality of the 4 chapters in this book is outstanding.

The first contribution, by Potter and Lewis, deals with reversed-phase chromatography of proteins. It follows a similar chapter that was presented in Volume 3 but stresses high-resolution aspects of biopolymer analysis. The chapter is short and does not dwell on theory. Instead it summarizes operational variables that have to be dealt with when large molecules are involved. Chapter 2 deals with one of the most important critical areas in HPLC, the development and characterization of various packing materials. Floyd and Hartwick introduce the concept of selectivity at a fundamental level and then present a concise description of the various types of interaction that can be exploited to optimize a separation. Mechanistic studies are presented along with applications. Chapter 3 deals with electrochemical detectors in HPLC. In his 103-page contribution. Shoup starts out with electrochemical principles and follows up with the most detailed and thorough coverage of design principles and operating characteristics for electrochemical detection that is available to date. Some 300 references are listed. The chapter by Snyder et al. also deals with the separation of large separation processes and discusses in great detail mechanisms that can be exploited in terms of adjustment of stationary-phase and mobile-phase parameters. This chapter contains a significant amount of theory. An attempt is made to summarize the topics as they are discussed. Special emphasis is placed on optimization and a large number of applications is presented. A comparison of RP, IEC, and SEC is shown in the appendix. This is a particularly informative method to highlight the differences between these techniques in physical terms.

There is very little that can be criticized in this book. It it timely and can be highly recommended. It is particularly important for scientists that deal with biomolecules.

**Wolfgang Bertsch,** *The University of Alabama*

**Surface and Interfacial Aspects of Biomedical Polymers. Volume I. Chemistry and Physics.** Edited by Joseph D. Andrade (University of Utah). Elsevier Science Publishers: New York and London. 1985. $69.50. XVI + 470 pp. ISBN 0-306-41741-3

This is an excellent text covering many aspects of surface and interfacial characterization of polymers, specifically those associated with biomedical applications. In fact, this title is somewhat restrictive in that anyone who is interested in the surface chemistry and physics of polymers, be they biomedically related or not, will find this text extremely useful. The text is intended as an introductory text for advanced undergraduates and graduate students as well as a reference text for those who wish to practice in the area. It is somewhat ambitious with respect to use as an advanced undergraduate text. However, the way it is laid out and the material presented will make it very useful for graduate courses. The text is a series of 13 chapters written by various authors. The chapters cover a large number of subjects concerning the characterization and measurement of polymer surface characteristics. Despite the fact that it is claimed to concern biomedical polymers, there is no discussion of biomedical applications whatsoever. The text is extremely well laid out; despite the fact that there are multiple authors, there is a high degree of continuity through the text. Eight of the chapters are authored or co-authored by Dr. Andrade. Additionally, he has obviously taken considerable care in organizing the text such that even those chapters not co-authored by him are of similar uniform format and possess approximately the same degree of theory and applied information. Each of the chapters contains both introductory material and experimental description as well as key results found in the area. There is also a considerable amount of basic data.

An introductory chapter thoroughly reviews the purposes of the text. One particularly useful section of this chapter contains lists of key textbooks and monographs in the area, recent symposia proceedings that are related, a list of important serials and publications, and finally societies and professional organizations of interest. This is an rather useful set of information for those people who are just beginning to become familiar with this field. While these listings may make the book dated rather rapidly, their inclusion illustrates that the authors truely wish to introduce the reader to all aspects of the field. The first several chapters of the book are devoted to polymer surfaces and their dynamics as an introduction. The next chapters are concerned with the nature of polymers and their given surface properties. Model polymers for probing surface characteristics are presented with considerable technical detail. Polymer layers and multilayers as model surfaces are described. The book then contains a series of chapters concerning instrumental analyses of surfaces including discussion of surface infrared spectroscopy, contact angle and interfacial energetics, interface acid base charge transfer properties, surface Raman spectroscopy, and interfacial electrochemistry of biomedical surfaces. Finally, several chapters are included to present related topics such as a discussion of the surfaces of graph and block copolymers and also interfacial tension and amorphous polymer–water interfaces.

Thus the textbook presents a remarkably complete description of polymeric surfaces, the methods used for probing them, and key results in many areas that are directly relatable to or important for biomedical applications of polymers. In summary, this textbook is an extremely complete, well-written, and thorough discussion of the subject. It should be on the shelves belonging to anyone interested in biomaterials and biomedical polymer surface properties and, in fact, is of considerable utility to those people who are interested in any surface characteristic of polymers.

**Kenneth J. Himmelstein,** *Allergan, Irvine, California*

**Spectroscopy of Molecular Excitons.** By V. L. Broude and E. I. Rashba (Academy of Sciences of the USSR, Moscow, USSR) and E. F. Sheka (Academy of Sciences of the USSR, Chernogolovka, USSR). Springer-Verlag: New York, Heidelberg, Berlin, Tokyo. 1985. ix + 271 pp. $48.00. ISBN 0-387-12409-8

This book is an important bridge between molecular spectroscopy and solid-state physics. It's appearance will, hopefully, draw attention to a hitherto little appreciated classical endeavor of molecular crystals spectroscopy.

Molecular excitons may or may not play an important role in the newly discovered high-temperature superconductors. They also may or may not play an important role in the nervous system. They certainly do play an important role in organic conductors, in the characterization of polymers, and in the primary process of photosynthesis. The discovery of molecular excitons, as well as their basic characterization, comes from work on molecular crystals, mainly from spectroscopic work.

Based on an earlier Russian version, this book is a beautiful exposition of more than two decades of work based, to an important extent, in the Soviet Union and in which the three authors played a major role. It is a very welcome addition to the international literature. In contrast to

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