Computer Software Reviews

Molecular Presentation Graphics. Version 3.0. Hawk Scientific System, Inc.: 170 Kinnelon Road, Suit 8, Kinnelon, NJ 07405. Price: $275.00. It comes with a copy protected disk but allows up to two backup copies to floppy or hard disk. Replaceable backup costs $25.00 with a proof of purchase.

This program works with IBM pc, XT, AT and its compatibles, HP 150, Dec mate and needs IBM color card or Hercules graphic card, a plotter with a maximum of four pens or H-P Laserjet or Lasejet+, printer (dot matrix, Epson, IBM), IBM 3812 page printer. The mouse is optional.

Molecular Presentation Graphics (MPG) is a structure drawing program specifically designed for chemists. Its purpose is to aid in the drawing of chemical structures and reactions. It does not adhere to chemical principles (see review: *J. Am. Chem. Soc.* **1985**, *107*, 6140; **1986**, *108*, 5044).

It is one of the most powerful and user friendly programs. All the commands are readily available on screen and the user is prompted what to do next or what is to follow. The document is very well written and comes in a small ring binder (~40 pages). It is easy to read and follow and is accurate. Although the manual provides necessary information, one could do without it equally well. It gives several useful drawing hints and a novice can take advantage in the initial use of the program.

When first started, the program has the screen divided into four basic areas: (1) a drawing area (occupies major portions of the screen), (2) below the drawing area is a series of eight labels or buttons which can be activated by function keys, (3) above the drawing area is the message area, (4) the top right of the drawing area is for mouse function labels and just below this area is for *X,Y* coordinates of the cursor. The screen displays tick marks to assist in the alignment of diagrams and this is very useful during screen scrolling.

The drawing area can be shifted eight horizontal pages (screens) to the left and thirteen vertical pages up. This allows no cut and paste requirements for a large layout. All the functions (or buttons) can be accessed with either function keys (F1–F9) or the mouse. The mouse makes the operation very easy and convenient. Several options are available with the mouse regarding the manner in which the commands are given to MPG. Without the mouse one is limited to using the keyboard. The cursor can be moved in slow, medium, or fast modes with the left, right, bottom, or top arrow keys on the numeric key pad or one has the option to create bonds of fixed (default) bond lengths. It should be pointed out that as one gets familar with various commands, the message area is more or less ignored by the user.

The first (main) screen prompts for a line, figure, text, edit, file, global, plot, and exit options. At will, each of these buttons will display another set of pertinent options. For example, one can draw a line in ten different formats (normal, dashed, dotted, forward, backward, bold dot, squiggley, heavy, arrow, and arc) that can be changed in its pattern (double, triple bonds, etc.), style, direction of arrow, line, or arc very easily. One can draw polygons (3–9 membered rings) and a benzene ring automatically or a custom drawn picture at any part of the screen. Ring fusion (any size to any size or spiro rings) and even creating quaternary centers are extremely easy, following the direction on the message area. Because of the "flip" command, mirror images of optical isomers can very easily be drawn. Also, prompts make sure that the structures have been placed at the desired position. If not, right away there is a chance to correct the placement. Figures can be rotated $^1/_8$ or $^1/_2$ size intervals (clock wise) and tilted to draw a variety of structures (e.g., sugars) conveniently. The "branch outward" command is very powerful and works at any line-end point, with a different result depending on how many bonds intersect at that point. The "approve and repeat" option allows entry into the same ring type multiple times without leaving the program.

To add the text, one has to compose a desired text (up to 78 characters) and then place where it is needed. The text entry allows one to specify which character is to be the reference character for the string. This allows placing the text left to right as well as right to left or centering the string for center labels. Text size is available in five different sizes. Superscripts and subscripts can be appropriately placed by using the top and bottom arrow keys in the text mode.

The editing capabilities are extremely powerful (change text or line or zone shift, resize, scroll, and redraw). One can change a single bond into a double bond or a double bond into a single bond, etc., with ease and without erasing. One of the most useful function is the "drag" (point or bond) to make three-D structures (e.g., boat and chair structures). The zone function is very powerful. One can move, delete, copy, keep, or highlight the entire drawing or a part of the drawing using the zone function. Also, MPG allows assigning a color to a specific line (e.g., highlighting the formation of a new C–C bond) (a color monitor is not needed). The program remembers up to approximately 1000 bonds, which are more than adaquate for most needs.

The files created are regular binary files. Created drawings can be listed on screen or a printer and can be loaded or added to the screen. However, in order to delete a file one has to use the DOS command which is available only after coming out of the program. However, this should not be a limitation. The MPG "reminder" feature counts the number of drawing commands entered and begins to remind at the main menu level if you have failed to backup. This would be appreciated should a power failure or some other disaster occur.

Plotting can be done on either vertical or horizontal paper of any size (8 × 11.5 or 11 × 17 in.). Plotting speed can be varied so that the plotting can be done directly on paper or a transparancy without the possibility of smearing the ink. Prior to the plotting, one can view (but cannot edit) the entire diagram on one screen, so that one will know in advance how the plot looks after actual plotting. By assigning a maximum size (in inches) to plots, the drawings will be scaled such that the standard bond length does not exceed that size. If the plot box is insufficiently sized the drawing will be automatically scaled down. The reviewer prefers the plotter over laser printers. Plotters provide better control for size and in placing the drawings at any part of the page and allow four different colors which make them convenient for preparing color slides.

The utility section provides a " convert" program that allows the convertion of files created by previous versions of MPG to the present 3.0 version. Also, it supports ASCII text files as well as files produced by the "WordStar" print command and "Displaywrite-3" files (which have been converted to .FFT format).

The menu displays an alternate character (greek characters, etc.) option, but in this version it is not available. Editing curves and circles is not ideal and needs improvement. One feature almost every chemist would like to see is hide-a-bond; unfortunately this feature is not available. Exiting the program without a disk in the primary disk drive (usually A) also causes the computer to lock-up, and in that situation, the only way to exit is cold or hot booting.

The 3.0 version of MPG has been considerably improved over previous versions yet it is compatible with the drawings created from the previous versions. It is very sophisticated yet simple to learn and use. It is a good value product for those who have a need for direct reproduction structures for a journal or have a need for high quality slides for overhead projectors. Since the program is menu driven, one will have no problem in using this package. A few minutes of experimentation with the program allows one to begin producing drawings without referring to the manual. As one becomes faimiliar with the program other features of logic and planning are appreciated. The reviewer's experience indicates that the drawing time for a complex synthetic scheme is close to or even shorter than the time necessary to draw the scheme manually. MPG satisfies most, if not all, of the chemist's needs. Customer service and support is excellent. Overall, MPG stands out as the best chemical drawing program that the reviewer has seen to date and it is recommended very highly.

Note Added in Proof. In version 3.2 of MPG, "alt.set" function allows the use of Greek characters. Editing of arcs and circles has been considerably improved. "Hide a line" function which was missing in the previous version has also been added. "Full screen zone" allows very easy reorganization of a large scheme. Zone rotation (in degrees) and new line patterns (open unfilled wedge, equal hatch, rivers line direction) have been included. In addition to the usual binary files, files can be created in HP-GL language which are useful for graphic export to commonly used word processors.

Muthyala Ramaiah, *Dow Chemical Co.*

chemFile and chemLit (IBM PC). By Dr. John Figueras. COMPress: A Division of Wadsworth, Inc., P.O. Box 102, Wentworth, NH 03282.

The software requires an IBM PC with 256K of memory, two disk drives or one disk drive and one hard disk, graphics board, and graphics monitor. Optional recommended equipment include a dot matrix printer, hard disk, Microsoft mouse and software, and Hewlett Packard series 7470A, 7475A, 7550A, or 748XB plotter with HP graphics language.

Chemfile and chemLit are file manager programs written for the IBM PC that accept two-dimensional chemical structures. In addition, chemFile accepts up to twenty user-defined data fields, while chemLit accepts free form abstracts. Structure input is not difficult and the structure entry tutor covers the essential points needed to get started. Cursor-key or mouse movement of the graphics cursor allows input of preformed three- to ten-membered rings (including benzenoid), functional groups, and single to triple bonds. Groups or bonds are easily added or removed for structures under construction. Fused ring systems can be generated rapidly, and previously defined structures can be recalled and modified. ChemLit allows the storage of chemical reactions and "knows" the difference between reactants and products. The marking of reaction sites of reactants and products allows the user to indicate additional search parameters. Care should be taken during structure input so that all substructures or fragments of molecules are consistently represented within a database, or it may not be possible for the programs to determine that they are identical during searches. Both programs allow the database to be queried in a flexible format by integral search units. ChemFile allows searches on multiple data fields, full structures, or structure fragments. ChemLit allows searches on keywords, text substrings, full structures, structure fragments, reactions, reaction starting material, or reaction products. Both programs allow cascading searches. If an initial search results in a large number of matches (hits), the hits may be subjected to additional searches that take much less time. Only the hits are subjected to the additional constraints producing a much smaller hit list. Defining a text search is very straightforward, while structure based searches are a little more involved. The online help facility is very useful for these cases. Once the search parameter(s) have been defined the database(s) are searched one entry at a time and the hit file written on each disk. The hit list may be subjected to further searches or displayed on the screen. On an IBM AT, a search takes about 0.3 to 0.5 s per structure, thus a full database, containing around 500 structures, could be searched in 3 to 5 min.

Hard copies of structures require either a dot matrix printer (draft quality) or plotter (publication quality). The programs allow the user to scale the size of the structure to a limited degree, but excessive reduction may result in distortions of the structure. This is not a major problem, however, because the program allows for the cancellation of all scale modifications and one then need only start the modifications over.

The programs were tested on an IBM AT with an IBM EGA adapter and appeared to run without errors. When they were tested on other IBM AT's and AT compatibles with compatible EGA adapters, varying degrees of structure corruption occurred upon storage.

In summary, chemFile should be very useful for storage and retrieval of structures and associated data such as melting point and identification numbers. ChemLit is better suited for storage of synthetic information due to the reaction storage capability. Structure input and search parameter definition is well documented and online help available. After reading the manuals, most people should find that the online help menus are all that is needed. The searching capabilities are good and rather fast. The amount of data that may be associated with a structure, while not large, should be adequate for most users. With the optional plotter, high quality hard copies are available for publications or slide masters and this in itself is a very good reason for package purchase.

Thomas E. Sorensen and James M. Cook, *University of Wisconsin—Milwaukee*

CLEOPATRA. Version 1.0. *C*hemometrical *L*ibrary: an *E*xtendable set *O*f *P*rograms as an *A*id in *T*eaching, *R*esearch and *A*pplications. Elsevier Scientific Software: 52 Vanderbilt Avenue, New York, NY 10017. Attention J. Tagler. List Price $675.00.

CLEOPATRA is a series of menu-driven modules designed as a teaching aid in Chemometrics. The package currently contains six programs covering the areas of sampling, monitoring, curve fitting, time series analyses (process reconstruction and autocorrelation), and fast fourier filtering. Additional modules have been planned and will be provided by Elsevier Scientific Software (ESS). For example, the first extension, comprising three modules covering Kalman filtering, Simplex optimization, and sequential analysis, is available for $420. Others are planned for factorial design, minimum spanning tree, detection limit, and lab simulation. In addition, new user-written programs (up to 249) can be easily interfaced to the existing driver program.

The CLEOPATRA package is provided on a set of three floppy diskettes and includes a user manual. Up to four copies of each diskette can be made under terms of the license. CLEOPATRA runs on the IBM family of microcomputers (PC, XT, and AT), equipped with at least 128K, one diskette drive (hard disk and printer are optional), DOS 2.0 or higher, and either interpreted or compiled BASIC. CLEOPATRA is also available for the Hewlett Packard (HP) 9845-B-(T), equipped with 186K, graphics and I/O ROMs, and HP-BASIC. The software package is supplied on HP cartridges. This review was conducted on the IBM version of CLEOPATRA.

Installation is not as straightforward as the user is led to believe by the ESS promotional literature ("...CLEOPATRA is extremely simple to use and requires no prior knowledge of any specific computer jargon."). This fact becomes rapidly apparent to the novice user when he/she encounters the installation instructions in the manual. The user is asked to select between an interpreted and two compiled BASIC versions of the same program (each version is on a separate diskette) *without* any discussion in the manual as to the difference between these versions (i.e., how to determine which version best suits you and your particular machine). This philosophy persists throughout the setup instructions—constant reference to the DOS manual is being made at just about every step, which will quickly result in an inexperienced computer user spending more time attempting to install the program then actually using it! Since one of the diskettes contains an interpreted version of the package, changes to the code by the user with a knowledge of BASIC can be made. A good description of the driver and its operation is provided for those users interested in adding their own programs to the package.

Operation of the program proceeded as described in the manual. Overall, the authors have made good use of graphics (no color). However, each module was found to be lacking in scope. For example, the curve fitting module only deals with the use of nonlinear regression in infrared spectroscopy. Similar treatment is also applied to the other five modules.

The manual, in general, is rather poor. The user is constantly being asked to consult outside handbooks on the subject in question; however, in most cases no suggestions or references are provided. A review of the subject matter that encompassed the examples demonstrated would have been a better approach. This would have made the relevance and usefulness of the examples clearer to the general user.

Although the package is designed for student use the overall price (and the ESS policy of no academic discounts) does not make this a very attractive teaching tool for either the student or the instructor.

Michael A. Pleiss, *SYNTEX Research*

PROPCALC. Siskiwit Bay Software Co.: 1603 E-2 Valley Road, Champaign, *IL* 61820. List price $45.00.

PROPCALC is a software package for calculating the physical properties of chemical compounds. It requires an IBM or compatible PC with 128K memory and works equally well from hard or floppy disk.

The program contains approximately 300 common chemical compounds divided into 19 libraries. Each library is made up of compounds containing the same number of carbon atoms. A list of physical properties is tabulated for each compound including molecular weight, boiling point, melting point, liquid density, and heat of vaporization. The program allows for the computation of vapor pressure, liquid viscosity, and vapor heat capacity as a function of temperature. Liquid activity coefficients and binary vapor–liquid equilibria curves may also be calculated. These calculations are performed quickly according to equations standardly found in handbooks and described in the user's manual. In cases where the information is not available, the execution stops and allows the user to return to the main menu.

The menu-driven format of PROPCALC makes the package simple to use. The software also contains routines which allow the user to create new libraries of compounds or edit the libraries already present. PROPCALC is a useful package for any chemist desiring quick calculations of the above properties.

P. A. Fleitz and C. J. Seliskar, *University of Cincinnati*

ASYST. MacMillan Software Company: 866 Third Avenue, New York, NY 10022. List Price: $1695–2195 (25% academic discount), depending upon package. A technical support plan, including access to software engineers and automatic updates of the package, is available for an additional $275/year.

ASYST is a sophisticated data acquisition and analysis software package expressly designed for engineers and physical scientists using an IBM-PC or compatible. It is not, however, for the faint-hearted. Rather, it is a high-level programming environment which requires a sustained effort to master and use effectively. Anyone who is committed to user-

friendly programs that can be implemented in a few hours of terminal time should look elsewhere.

ASYST consists of four modules. Module 1 consists of a graphics and statistics package. Data are input through one of several modes: by keyboard using either the self-contained editor or a special-purpose array editor, from an ASCII file using a free-format input, through the asynchronous (RS-232) port, or from one of the interface modules in real time (see below). The data can be edited, subjected to complex manipulations, and displayed graphically. Hardcopy is available on a printer or plotter using a variety of plotting formats, including arithmetic, logarithmic, and polar coordinates, as well as the usual bar graphs and pie charts. A windowing feature allows presentation of multiple graphics, e.g., decay curves and residuals, in the same plotting field.

Module 2 contains the analysis package. Complex curve-fitting functions are available. In addition, three-dimensional plotting is available, either through axonometric (perspective) or contour plots.

Module 3 is the data acquisition package. It provides software handling of the more popular analog input and output boards, including the Data Translation DT-2800 series, the Tecmar Labmaster, and the Keithley DAS 500 series. Buffered and nonbuffered I/O are supported.

Module 3 supports I/O using the General Purpose Interface Bus (IEEE-488). This software module, together with Modules 1 and 2, has become an industry standard for IEEE-488 interface communication and is often sold as a "value-added" product with digital multimeters, waveform generators, oscilloscopes, etc. A useful feature is the ability to graphically monitor analog input as it is received.

The most useful aspect of ASYST is that, as a threaded interpretive language, subroutines can be written, compiled, and executed interactively by use of keywords, which are executed whenever encountered. This allows the experienced ASYST programmer to develop programs that can be compiled and saved for use by others. Unlike FORTRAN, however, such routines are restricted to use with the original copy-protected master diskette. Experience in FORTRAN and BASIC is, unfortunately, more of a hindrance than a help, since differences from these languages can result in frustrating yet subtle errors. For instance, ASYST does not execute the last series in a DO loop. A more difficult problem is that use of arrays of variable length is almost impossible. Data are written in binary format, which makes communication with other programs difficult.

ASYST is written in a FORTH-like language. Its command structure has more in common with reverse Polish than FORTRAN. Thus all manipulations are carried out after loading variables onto the stack, and any manipulation of a stack variable removes it from the stack. The use of stacks has the single advantage that calculations such as fast Fourier transforms become very rapid. Also, matrix manipulations can be carried out by simple statements without using DO loops. However, coding of complex functions becomes very unwieldy. For example, the function $f(x) = x \exp(-xa)$ would be coded as follows:

```
REAL SCALAR A SCALAR X
: F(X)
DUP X A * NEG EXP * ;
```

Since ASYST does not use statement numbers, run-time error traceback is virtually nonexistent. The manual does not even provide a complete listing of error messages, and the error messages themselves are often uninformative. Given the subtleties of some errors, this can become maddening for complex programs.

The complete ASYST package comes with five bulky loose-leaf manuals. Each manual contains a tutorial and a glossary. The tutorials are a must, but use of the indices is difficult, since topics are not extensively indexed and a single topic may be contained in two tutorials and one glossary. This reviewer generally had three or four manuals scattered over his desk whenever he attempted to use ASYST, and use of a more compact manual would have been handy. Less general information about curve-fitting and other topics and more specific information about programming subtleties would have made the manuals more generally useful.

ASYST is supplied in three copy-protected diskettes. Although the program may be copied onto a hard disk, use of the original disk is required for program startup. ASYST will run on an IBM-PC or compatible with as little as 384 kB of memory, although 640 kB is suggested for more effective use. An 8087 math coprocessor is required, as well as an IBM graphics adapter or the equivalent. The IBM Enhanced Graphics Adapter is supported as well. A plotter is a must, although only HP7475 and HP7470 plotters are supported currently.

ASYST will be useful mostly to chemists involved in real-time signal acquisition, processing, and analysis, since the plotting features are readily available in some more inexpensive forms. A disappointment for spectroscopists is the lack of a deconvolution algorithm for analysis of time-resolved spectroscopic data.

Laren M. Tolbert, *Georgia Institute of Technology*

Book Reviews

Methods in Enzymology. Volume 130. Enzyme Structure (Part K). Edited by C. H. W. Hirs (University of Colorado Medical Center) and S. N. Timasheff (Brandeis University). Academic Press, Inc.: Orlando, FL. 1986. xxiii + 587 pp. $70.00. ISBN 0-12-182030-0.

In order to have a complete understanding of how an enzyme or a protein functions and how this function is regulated, it is necessary to know its three-dimensional structure. Additionally, conformational changes occurring during protein–ligand association and the catalytic process are intrinsic to the overall mechanism. This volume details methods for evaluating protein structure in solution and methods for evaluating structural changes induced by protein binding.

The first section of 9 chapters is devoted to macromolecular assemblies and includes methods for assessing protein self-association, methods for evaluating DNA–protein interactions, and methods for determining the thermodynamic parameters for protein–ligand association. The methods described include a number of sophisticated physical techniques such as differential scanning microcalorimetry and small-angle neutron scattering. The second section of 7 chapters concentrates on optical spectroscopic methods for determining protein secondary structure, including magnetic circular dichroism and Raman and ultraviolet resonance Raman spectroscopy. In addition, a chapter on resonance Raman determination of ligand binding to metal centers is included. Conformational transitions in macromolecules constitutes the topic for the third section of 7 chapters. Within this section, the reader will find discussions of the effects of electrostatic interactions on protein conformation and conformational stability, fluorescence and circular dichroism methods for determining the kinetics of protein conformational transitions, and a calorimetric method for measuring the kinetics of lipid-phase transitions.

This volume is a valuable compilation of many recently developed, sophisticated methods for determining protein solution structure and structural transitions. In addition to their detailed presentation of the experimental methodologies, most of the chapters include sufficient discussion of the theoretical aspects of the topic. However, many of the techniques described require sophisticated instrumentation not generally available.

Carol A. Caperelli, *Fox Chase Cancer Center*

Methods in Enzymology. Volume 131. Enzyme Structure (Part L). Edited by C. H. W. Hirs (University of Colorado Medical Center) and S. N. Timasheff (Brandeis University). Subedited by R. L. Baldwin (Stanford University School of Medicine). Academic Press, Inc.: Orlando, FL. 1986. xxiii + 653 pp. $69.00. ISBN 0-12-182031-9.

This volume continues the series on methods for studying protein structure and dynamics. As with the previous volumes in this series, this volume also concentrates on physical methods.

The first section of 14 chapters deals with the subject of protein folding. It is concerned with both the dynamic and the structural aspects of this topic. A number of methods that have been developed to study the kinetics, and thermodynamics of protein folding are described, including microcalorimetry and amide proton exchange. There is also considerable discussion of methods used for the detection and characterization of folding intermediates. Some of the newer approaches to these problems that have been included in this section are the use of cryosolvents at subzero temperatures and the use of mutant proteins. The application of many of the approaches that have proved useful in studies on monomeric proteins has been attempted with oligomeric systems.

Structural dynamics and protein mobility is the subject of the second section of 10 chapters. This section is concerned with what might be termed "microscopic" aspects of protein dynamics. That is, attention is focused on small amplitude changes rather than on gross structural changes. Among the methods that are discussed are nuclear magnetic