Computer Software Reviews

Molecular Mechanics Package (MS-DOS Computers). By J. J. Gajewski and K. E. Gilbert. Serena Software: Box 3076, Bloomington, IN 47402. List Price $100.

This package consists of three programs: a structure input program (STRPI), an energy minimization program (MMPMI), and a structure drawing program (MDRAWI). The structure input program sets up a coordinate file for energy minimization with Allinger's MMP program. The drawing program allows one to graphically view the output from the energy minimization routine and obtain a hard copy of the structure. Taken together, these programs provide easy access to molecular modeling on a PC.

The programs require additional hardware and software in order to run on a standard IBM-PC. The MMPMI program requires at least 550K of memory along with an 8087 math coprocessor chip. A full 640K of RAM is recommended. A smaller version of the program, which will operate with 512K of memory, is available. A hard disk is not required but is recommended for recompiling the program, or if large outputs are expected. The drawing program requires a graphics card and a Tektronix emulator program. PC-PLOT (Microplot Systems Co., 659-H Park Meadow Road, Westerville, Ohio 43081, $100) is recommended. This program supports a wide variety of graphics boards. The graphics card may be used during structure input but it is not required. Graphics is also not required for energy minimization for which a detailed output may be obtained.

The structure input is based on a modified version of a structure input program for MM2 developed by R. M. Jarret and M. Saunders. Input is very simple and consists of entering bond directions from one heavy atom to another using U (up), D (down), L (left), R (right), I (in), or O (out) commands. In graphics mode, a picture of the molecule is constructed as each atom is entered. Corrections may be entered during the graphics mode. A file record (STRP.INP) of the input (u,d,l,r,i,o) is also produced. Hydrogens are automatically entered upon completion of the structure. One may then enter instructions for restricting the motion of atoms in the *X*, *Y*, or *Z* direction or for using the dihedral angle driver. After completion of the input, a picture of the molecule may be displayed. The structure can be rotated and viewed in stereo.

Besides the normal MM2 atoms, the program allows input of several special atoms. These include radicals, carbocations, carbanions, ammonium ions, oxy anions, transition-state atoms (carbon, hydrogen, and boron), as well as several others. (Fifty atom types may be included.) Many of the constants for these atoms are still experimental but relative results from the minimization process should be qualitatively correct. For transition-state atoms, a fractional bond order between bond-breaking and bond-making atoms must be input. The STRPI program then automatically calculates and appends the appropriate constants to the input file. This feature greatly simplifies the input process.

Examples of input sessions are included in the documentation on the disk. A help section is also available within the program. Although entry is straightforward, it is a good idea to look at a model of the structure and plan the input before hand. Errors in entry may cause the program to fail. If mistakes are made, or additions or deletions are required, the STRP.INP file may be edited using a word processor and reentered into STRPI.

The energy minimization program is an expanded version of MM2 (QCPE 395) and MMPI (QCPE 318) written by N. Allinger. Several generalized parameters from MODEL (C. Still) have been added along with the ability to handle carbocations, anions, radicals, and transition-state atoms (carbon, hydrogen, boron). The transition-state atoms allow one to model pericyclic reactions (i.e., Cope rearrangements, ene reactions, etc.) and hydroboration reactions.

The IBM-PC version runs between 10 and 15 times slower than the VAX-11/780. The ready availability of a PC often more than compensates for the speed of the larger computers. The minimization process may take from a couple of minutes to several hours depending upon the complexity of the structure (100 atoms maximum) and the number of options used. Surprisingly, an IBM PC-AT is only about 20% faster than an IBM PC-XT. Output consists of a coordinate file for input into the drawing program, a coordinate file for input into MMPMI, and a data output file. The later provides all geometric and energetic calculations.

Documentation on how to run the MMPMI program is provided on the disk. Full documentation is also available, but this is not required unless you want to change constants or use some of the special features of the program. Reviews of molecular mechanics calculations are available (for example, *Molecular Mechanics*; Burkert, U., Allinger, N. L.; ACS Monograph 177, American Chemical Society: Washington, DC, 1982, or *A. Handbook of Computational Chemistry*; Clark, T.; Wiley-Interscience, New York, NY, 1985).

Although all energy parameters, coordinates, distances, etc., are produced in the output file, the graphical output program MDRAWI is extremely helpful. The graphics are acceptable on a normal color monitor but are excellent when a high-resolution graphics board is used. Using an IBM-Enhanced Graphics Adapter provides 16 colors of superb high-resolution display. In the later case each atom type may be represented by a different color. With a normal IBM color card only a monochrome display of the molecule is available.

The MDRAWI program provides a menu of several options for viewing the molecule. The molecule may be rotated in *X*, *Y*, or *Z* and drawn in stereo. The later feature greatly aids in visualizing the molecule. All or selected hydrogens may be added and van der Waal's radii drawn. Heavy atoms or hydrogens may be numbered. The depth perception, size, stereo separation, and van der Waal's radii may be changes. A zoom option allows a portion of the drawing to be enlarged. Geometric features such as distances, bond angles, and dihedral angles may be queried. In the later case, a proton–proton coupling constant is calculated. High-resolution picture files (mono or stereo) may be generated for plotting in monochrome or color by using the Microplot software. Options are also available for producing ORTEP and MNDO input files although these may need to be modified by the user.

The graphical output uses standard Tektronix routines. This means that real time rotations of the molecule cannot be performed since the screen must be erased before it is redrawn. However, structures are drawn fast enough so that this is a minor inconvenience. Another minor problem is that keyboard input may not be echoed on the screen with certain graphics boards (the IBM color card works fine). In this case, entry must be carefully done to avoid mistakes. Although most errors are trapped, the program will sometimes fail if the wrong data are input.

In addition to the molecular mechanics data, MDRAWI can be used with MNDO and MOPAC files.

Using a computer for molecular modeling can lead to observations which are not obvious from simple models. Just as with simple models, one may be led astray by the numbers provided by the computer. For example, the program may find local minima which do not represent the desired conformation. This "problem" is also a benefit since it allows one to compare energies of various conformations. Qualitative predictions of relative energies of epimers are usually correct. However, one must be aware that many of the constants are experimental and that generalized constants may have been used.

The program is well done and should meet the needs of most users. The authors have incorporated several features suggested by users and are continually improving the program. As with any program, there may be features which are not needed or are lacking for an individual user. The source code (FORTRAN) is available and may be modified. At present, the graphics portion must be compiled with Microsoft Fortran version 3.2. The latest version of Microsoft Fortran (3.3) will fail to give graphics output when used with the Microplot terminal emulator. Future versions of the software should correct this problem as well as the keyboard echo problem mentioned above.

In summary this software is easy to use and provides a complete package for powerful molecular modeling. The ability to model the many added atoms and transition states is a very attractive feature. The program has been used by students with little or no knowledge of MM2 or the IBM-PC with little difficulty after a short demonstration.

M. Mark Midland, *The University of California, Riverside*

Sci-Mate Software System. Institute for Scientific Information: 3501 Market Street, Philadelphia, PA 19104. August, 1985. List price $399.00 per component (10% discount when purchasing all three; 5% additional academic discount when purchasing all three).

The Sci-Mate Software System has three components: The Searcher, which is designed to provide menu-driven searches of online databases, The Manager, which enables creation and manipulation of data files, and The Editor, which will not be reviewed here. Each of the Sci-Mate components may be purchased and used independently, but the system is designed to allow easy access to common files.

Two versions of the Sci-Mate System are available: one for systems

using PC/MS DOS 2.0 or higher (IBM and IBM compatibles with or without a hard disk) and one for any CPM/80 operating system using 8-in. diskettes. The second version can be downloaded commercially to 5.5-in. diskettes for other CPM/80 operating system computers, such as Apple or KAYPRO, provided hard disk capacity is available. The reviewer used an IBM AT with hard disk. The total number of files is limited by the length of the files, the size of records in files, and disk capacity. For example, on a 512K disk about 900 records of 500 characters each may be stored. Any printer may be used to print records, labels, and columnar reports from the Manager, or to print hit lists from the Searcher. Any manual or autodial modem may be used to establish data communications, but only Ventel MD212-Plus, Cermetek 212A, Hayes Smartmodem 300, and Hayes Smartmodem 1200 are dialed automatically by the program. Installation of the Manager and Searcher proved to be straightforward and well documented for standard hardware and default settings. The reviewer encountered difficulty, however, when installing a modem at the non-standard port. While the Installation Manual did not offer a solution to the problem, the Sci-Mate service representative was able to supply the necessary hardware specification values. The Sci-Mate System may be used only by the purchaser and his employees; a single backup copy of programs may be made in case of disk failure.

The Sci-Mate Searcher acts as buffer between the user and an online database, enabling the user unfamiliar with a search language to conduct a search merely by making appropriate menu choices. Supported databases are shown in Table I. Users of the program must have an account with individual databases in order to enter the database and conduct searches. For those data files supported completely (Table I) the user need not know online datafile numbers, the fields available for search, or the syntax of the search statements. For new or unsupported datafiles (such as CA 1967–present in DIALOG) the user must supply file numbers and know which fields are available; however, the search is still aided by a series of prompts and menu choices. The Searcher also offers the option of switching to a suspended terminal mode or to the native search language before or after the data connection has been established.

For fully supported autodial modems the Sci-Mate Searcher dials the network (or directly to the online database), makes the connection to the database, optionally enters the necessary password(s), and enters the preselected user file. (For manual or other autodial modems the initial telephone connection must be made by dialing from the phone or keyboard.) Once online, menus prompt the user to construct a search statement, conduct a search, send or save a search statement, or browse a file. After a successful search the user can view, print, or store hits from the search into a file for later use. (Copyright restrictions prohibit storage of hits from some databases. Purchasers of Sci-Mate may download ISI files for personal use only.) The user may also enter another file within the same database, switch to the native search language while retaining the option to download (save) retrieved records, or log off the database. A tutorial for each database provides a useful, but fairly expensive introduction to Searcher online options.

The most useful feature of the Searcher is the ability to create search criteria before establishing a data connection. With this option, the user can create search statement(s) at his leisure. Once the online database file is entered, the search(es) are conducted automatically. The user is then returned to the online menu to manipulate retrieved records or to conduct further searches. Creating search statements offline and then printing or storing retrieved data for later viewing can save considerable online time, and hence money. A search statement may include multiple terms connected by boolean operators, two words with specified proximity, truncated word(s), and any number of terms, as permitted by the database. Stored hits from the Searcher can be accessed from the work file of the Manager, or from any ASCII software.

The Searcher is a very useful aid to online searching: novices can quickly learn to perform searches, and users of all experience levels can increase their online search efficiency.

The Manager consists of user files (which may be optionally formatted by previously created templates) and a work file. Records in a user file are like information in an index card file or Rolodex—for example, one file might contain an index of preprints a chemist has, another file the names and addresses of colleagues. Records may be "flagged" or marked to indicate their current status, such as whether a given preprint is on loan. Records in user files may be entered, edited, and deleted from the keyboard or transfered from the work file. The files may be searched or sorted, and files or parts of files may be displayed, printed, or moved to the work file. A user file may be used to create a columnar report including the status of any flags, and a file that is appropriately templated can be used to print labels. The work file can contain records copied from user files, saved by the Searcher, or retrieved from outside software files. Work file records may be reformatted, sorted, stored in old or new user files, or accessed by software outside the Sci-Mate System.

Table I. Sci-Mate Databases and Fully Supported Data Files

database	ISI data files	other supported data files
BRS	SOC SCISEARCH 1977–	ABI/INFORM 1971–
	SOC SCISEARCH 1972–76	BIOSIS PREVIEWS 1978–
	ARTS & HUMANITIES SEARCH	CA SEARCH 1977–
		COMPENDEX 1976–
		ERIC 1966–
		MANAGEMENT CONTENTS 1974–
		MEDLINE 1979–
		NTIS 1964–
		PSYCINFO 1967–
		CA SEARCH TRAINING
DIALOG	SCISEARCH 1974– (in four files)	ABI/INFORM 1971–
	SOC1AL/SCISEARCH	BIOSIS PREVIEWS 1981–
	ONTAP SCISEARCH	CA SEARCH 1982–
	ONTAP SOC1AL/ SCISEARCH	COMPENDEX 1970–
		ERIC 1966–
		MAGAZINE INDEX 59–70, 73–
		MANAGEMENT CONTENTS 1974–
		MEDLINE 1980–
		NTIS 1964–
		PSYCINFO 1967–
		WORLD PATENTS INDEX 1981–
		ONTAP ABI/INFORM 80–81
		ONTAP BIOSIS PREVIEWS
		ONTAP CA SEARCH
		ONTAP COMPENDEX
		ONTAP ERIC
		ONTAP MAGAZINE INDEX
		ONTAP MEDLINE
NLM	none	MEDLINE 1983–
ORBIT	none	ABI/INFORM 1971–
		CA SEARCH 1982–
		COMPENDEX, 1970–
		ERIC 1966–
		MANAGEMENT CONTENTS 1974–
		NTIS 1977–
		PSYCINFO 1967–
		WORLD PATENTS INDEX 1981–
		CA SEARCH TRAINING
		WPI TRAINING
QUESTEL	INDEX CHEMICUS ONLINE	CA SEARCH 1982–

The Manager also comes with a tutorial to familiarize the user with its features. Even after completing the tutorial, however, the Manager can be difficult to use. The large number of menus is confusing, and the program does not indicate how many levels the user is removed from the main menu. Some menu choices incompletely describe its subsequent menu: for example, the option to "Select/Create Another USER file" leads to the menu that allows the user to delete user files, or to specify a different disk drive, in addition to the stated options. The file name must be reentered from the keyboard each time the file is accessed, unlike some other software packages in which the desired file may be chosen from a list of files by using a cursor. A user file may not be viewed or loaded to the work file directly; instead, a search requiring several additional keystrokes must first be conducted and the records retrieved by the search manipulated further.

Though cumbersome to use at times, the Manager is well documented in the easy to read Manager Manual. In addition, descriptive help files may be accessed from any Sci-Mate menu, and a single keystroke enables the user to return to the previous menu at any time. The Manager does perform its stated file manipulations adequately and is adaptable to large and small files of records of variable size.

The reviewer has used the Manager primarily to manipulate files

provided by the Searcher, but perhaps an extravagance for this use alone. A chemist, industrial or academic, who has a large number of files which he accesses frequently might find the Manager a useful index. The Manager is adaptable to a variety of additional filing purposes, such as cataloging chemicals or equipment in a laboratory.

Kimberley Cousins, *The University of Texas at Austin*

MacDraft. Version 1.1. 1985. By Leonard G. Barton. Innovative Data Design, Inc.: 1975 Willow Pass Road, Suite 8, Concord, CA 94520. List price $250.00.

MacDraft is supplied on a copy protected disk with a backup available for a $10.00 fee. Any number of copies of the master disk may be made (e.g., so that different systems can be incorporated) but the boot operation requires the insertion of the master disk.

MacDraft is an object-oriented drawing program for the MacIntosh which is styled very much in the fashion of MacDraw (see review: *J. Am. Chem. Soc.* **1985**, *107*, 6140). In the great majority of its functions, MacDraft works identically with MacDraw and the reader is referred first to that review since this one will concentrate only on the areas where the two programs are different.

Perhaps the most obvious feature of MacDraft absent of MacDraw is the ability to rotate objects through a full 360° turn, in 1-deg increments. This feature permits the ready alignment of rings of different size (e.g., 5 and 7) without freshly creating one or the other for this purpose. The facility with which this operation can be carried out is unfortunately counterbalanced by the absence of the ability to view complete objects as they are being moved. Thus, when letters are created and moved onto structures, repeated attempts must be made to place them precisely. This drawback appears to affect only characters, for when objects such as polygons are moved they are outlined by their perimetries. Thus, such objects can be set and aligned exactly in relationship to others.

MacDraft has a zoom feature which is very useful. It can be used to zoom in and out of various views to encompass either a larger or a smaller portion of the current document. Unlike MacDraw, the zoom in feature prompts with a rectangle for the actual area of the document that is to be enlarged. In addition, the very most magnified view represents a considerably smaller area of document than available with MacDraw and thus allows for much greater precision in alignment. MacDraft also has a feature that allows a series of objects to be placed symmetrically disposed along a line. This facilitates the generation of layouts with multiply repeated subunits.

MacDraft has a free-hand drawing feature that is more versatile and very much more useful than that found in MacDraw. In the latter program, the creation of a free-hand object is an all or nothing operation as no corrections can be made. In MacDraft, the object can be edited as it is formed by simply backing up. This is useful for creating such features as the wavy lines indicating unspecified stereochemistry. One final significant difference is noted in that unlike MacDraw, MacDraft is incapable of changing the size of a set of objects which have been grouped. This represents a significant drawback for the coreation of a free-hand structure like that illustrated in the MacDraw review.

Overall then, while the two programs are quite similar in their operation, there are unique features in each that are useful. In the case of MacDraw, it is particularly noteworthy that there is the ability to rotate objects by 1-deg increments and to zoom in on a very highly magnified subsection of a document.

Information can be transferred from MacDraft to MacDraw and vice versa, using either the scrapbook or the clipboard. However, the method of storage appears to be somewhat different and MacDraw documents cannot be opened by MacDraft.

James K. Whitesell, *University of Texas*

PC-PLOT. MicroPlot Systems: 659-H Park Meadow Rd., Westerville, OH 43081. List Price $99.00.

PC-PLOT is an asynchronous telecommunications program which allows an IBM PC with a modem to be used as a terminal to access online systems. PC-PLOT emulates a Tektronix 4010 (PLOT10) terminal, so it can be used as a graphics terminal for the CAS ONLINE database on STN International.

PC-PLOT comes on a Distribution Master disk, with a 96-page user manual. You copy this disk to produce your working disk. The manual is self-explanatory and has answers to most questions that arise. One section lists compatible computers, graphics boards, and printers that have been tested by MicroPlot. In the setup procedure you identify the terminal, graphic board, printer, and communications protocol (full duplex, 7 data bits, 1 stop bit, and even parity). If the modem (such as Hayes 1200) has autodial capability, a phone directory can be set up in PC-PLOT.

PC-PLOT has a set of "local commands" for functions such as clearing the screen. These commands are listed on a HELP menu (accessed by pressing the ALT and H keys).

Graphic Input (GIN mode) is available to DRAW a query structure or select from a MENU. Pressing the cursor arrow keys moves the cursor one pixel at a time. Your can speed up the cursor movement by pressing the Scroll Lock; then the cursor jumps 8 pixels at a time. An optional mouse may be used instead of the cursor arrow keys for drawing.

Graphic structures are clearly displayed on the screen. When they are printed (on a dot-matrix printer such as Epson FX-80), the structures print out sideways and require about 2 min per page.

When doing text searching, you can set the terminal in alpha mode and set the printer for slave-printing. Text queries can be uploaded. Text and graphic sessions can be downloaded to disk.

Daniel E. Nemzer and Matthew J. Toussant,
Chemical Abstracts Service

GriffinTerminal 100. Metaresearch Inc.: 1100 SE Woodward, Portland, OR 97202. List Price $99.00.

GriffinTerminal 100 (GT-100) is a telecommunications program which allows an Apple Macintosh with a modem to be used as a terminal to access online systems. GT-100 emulates a Tektronix 4010 (PLOT10) terminal, so it can be used as a graphics terminal for the CAS ONLINE database on STN International.

GT-100 comes with very complete printed documentation: a detailed table of contents and pictures of the menus used to set up the software to match the host computer. The documentation also comes in a sturdy binder that allows room for updates or notes.

To use GT-100, load the diskette and OPEN the program by double-clicking the mouse with the screen pointer on the Griffin icon. A setup menu is displayed at the top of the screen. These items are selected to use CAS ONLINE or similar online services: FILE (stop print, stop receive), GRAPHICS (true scale, enable screen, enable scroll), MODE (text transfer, remote), SETTINGS (1200 baud, 7 data bits, 1 stop bit, full duplex, even parity), FONT (80 column std). Now dial the telecommunications network and login.

To download, select the FILE option from the menu. By using the mouse, select "Receive Next from Host", and downloading begins. To stop downloading, select the same menu and use the mouse to select "Stop Receive". To clear the screen, select "Clear" on the GRAPHICS menu.

Graphic Input (GIN mode) is available to DRAW a query structure or select from a MENU, using the mouse. Graphic structures are clearly displayed on the screen and can be printed (on a dot-matrix printer).

Daniel E. Nemzer and Matthew J. Toussant,
Chemical Abstracts Service

Tekalike. Version 2: 11/85. Mesa Graphics: P.O. Box 600, Los Alamos, NM 87544. List price $240.00.

Tekalike is an emulator for the Tektronics graphics terminal which allows the user to integrate graphics from a mainframe computer into the Macintosh environment. Specifically, it emulates the Tektronix 4010, 4012, 4014, and 4016 terminals and this it does extremely well at a fraction of the cost of a complete Tektronix terminal. Tekalike is designed specifically for the Macintosh but is also available for the Apple Lisa and Apple II computers. The only requirement is one of the aforementioned and some means to communicate with the host computer.

Tekalike has no particular chemical application but offers the Macintosh owner a unique software package to convert his computer into a complete graphic and text terminal while taking advantage of the unique features of the Macintosh. Two related applications are the accessing and viewing of plots of Cambridge crystallographic data and the performance of molecular mechanics calculations. Of course, these capabilities are not specific to these applications but represent the two prominent features of this software—the ability to input data to graphic programs and to view plots from mainframe software. Limitations to this capability arise, not due to limitations in the software itself but rather from limitations in the Macintosh. The resolution of the screen is significantly less than that of a Tektronix. Plots of curves tend to be approximated by a series of noticeably jagged lines.

Since Tekalike allows you to print out the screen, it is possible to obtain the equivalent of a "rough draft" of a graphics output using the Imagewriter. This feature can be used to advantage for instance with molecular mechanics calculations where it is not necessary to obtain a high quality plot but some sort of hard copy is essential. The screen image can be printed quickly, conveniently, and inexpensively, providing such verification. This is also a real advantage to someone who lacks access to a plotter. Moreover, the picture can be printed on the Laserwriter which the Tekalike supports. This provides the opportunity for a very good quality hardcopy, significantly better than can be obtained on the Imagewriter alone. Tekalike also allows you to reduce or enlarge the picture (10–500%) for printing. This software also supports the following plotters: Apple 410, Hewlett Packard 7470A, 7475A, and

7550A, and Houston Instruments DMP29, PC695, DMP51, or DMP52. When tested with a HP 7475A plotter, Tekalike performed superbly. Graphics which were saved could be plotted at various speeds and with control over the page arrangement and size. The quality was noticeably superior to the plot as seen on the screen, giving results comparable to plots directly from the mainframe. The only requirement is that the plotter use the RS-232 interface protocol. (It is not possible to use a plotter with an HP/IB configuration.)

Tekalike's ability to integrate graphics from a mainframe into the Macintosh environment is particularly elegant in that it is possible to display graphics from a mainframe, save it on a disk, then view it at any time while no longer in communication with the host computer. The software is intended to provide the capability to take graphic output and convert it into a Macpaint document. (Note that the Macpaint software is not part of Tekalike and must be provided by the user.) This task Tekalike accomplishes easily, but because of the limitations of the screen resolution, the results may be disappointing, depending upon the graphics, as the resulting Macpaint documents are often not of sufficient quality to paste directly into word processor documents.

A graphic recording can also be converted into a Macdraw document (Macdraw not included). The image can be scaled to fit on one Macdraw page using the "Shrink" feature. If this is not used, then a multiple page document is created. Once the document has been transferred, it is possible to rearrange the graph as elements can be grouped and moved about, thus allowing editing of a plot or picture without having to change the generating program. However, the information is not converted into true Macdraw objects.

There is a "Zoom" feature which allows a closeup of any region of the display. This works extremely well when used with a good quality graphic output stored on disk. Zooming provides the opportunity to plot specific areas without modification of the plotting software, a real time saver.

Tekalike will support standard screen editors such as the Vax Edit/EDT editor using VT100 commands. It can be used with or without a keypad, although the latter is more convenient. With the Vax editor, the backspace key sends the cursor back to the beginning of the line while moving back one space requires a control command.

A text stream can be recorded and later viewed with Macwrite (not included). The text is saved as Geneva typeface and can be edited as any Macwrite document. This allows the opportunity to incorporate text output directly into a word-processed document.

Tekalike can be used to dial another computer with either a rotary or touch tone phone with the number saved. All the communications parameters such a baud rate (300 to 19200), parity, handshake, local echo, auto line feed, and bits per character can be set and saved for future use. When interacting generally with host, your computer can be set as an ANSI terminal with adjustable character size and margin settings. In this format text scrolls, but when a graphic output is sent by the host, the terminal automatically switches to Tektronix mode. After the graphs have been viewed, the terminal can be switched back to the ANSI mode. Even though the screen lacks color capability, color plots can be realistically previewed with different colors represented by eight different shading patterns.

A real advantage of this software is that it enables the user to input graphical data directly to a mainframe computer using the Macintosh Mouse. For example, drawing molecular structures for Molecular Mechanics calculation is greatly simplified.

The accompanying manual is very good if you are familiar with the Macintosh. Since all operations are menu controlled, a few hours with Tekalike is all that is necessary to learn its features. Examples of all operations are provided in the manual as well.

John Pojman, *The University of Texas at Austin*

*Book Reviews**

Folk Medicine. The Art and the Science. Edited by Richard P. Steiner (University of Utah). American Chemical Society: Washington, DC. 1986. viii + 223 pp. $22.95. ISBN 0-8412-0939-1. (Also available in paperback: ISBN 0-8412-0946-4.)

This book appears at a time of renewed interest in folk medicine and will provide interesting reading for the layman as well as physicians and researchers.

The first seven chapters are devoted to the medicinal plants of specific areas or cultures. These are Aztec sources of Mexican folk medicine, Zuni Indian medicine, medicine of India, and medicinal plants of Fiji, Papua-New Guinea, Australia, and Africa. Attempts are made to evaluate plants on the basis of efficacy or laboratory analysis. The antithrombotic activity of garlic is the subject of Chapter 8. This is followed by a discussion of the scientific basis of the therapeutic effects of ginseng. The next three chapters describe Chinese medicinal plants. The last two chapters are concerned with the bioactive components of Zingiberaceous and Zizyphus plants. The last seven chapters emphasize the isolation and identification of specific bioactive compounds. References are included.

M. C. W. Smith, *Ann Arbor, Michigan*

Chemical Demonstrations: A Sourcebook for Teachers. By L. R. Summerlein (The University of Alabama at Birmingham) and J. L. Ealy, Jr. (The Hill School). American Chemical Society: Washington, DC. 1985. ix + 190 pp. $19.95. ISBN 0-8412-0923-5.

The book contains 108 teaching demonstrations conveniently bound, presumably for laboratory use, in a ring binder format.

The authors do not specify the educational level for which the demonstrations are designed other than to suggest their use in an introductory program. This may be quite consistent with their admonition, perhaps to college teachers particularly, that often "we overlook very effective demonstrations because they are so simple". Most of the demonstrations seem appropriate for audiences of different ages. In addition to being simple and easy to understand, the demonstrations conform to the authors' criterion that demonstrations be fun.

I liked No. 42, Carbon as a Catalyst, which suggests that a sugar cube can be burned after being coated with cigarette ashes, and No. 85, The Surface Tension of Water, in which floated powdered sulfur sinks when the water surface is touched with one's finger.

Important to large group lecturers is the identification of some demonstrations which can be done in Petri plates and shown on the overhead projector. The comparative reactivity of several metals in a marked plate and the reaction of sodium with water and an indicator, as examples, project beautifully. Perhaps the crystallization of sodium acetate, demonstration No. 17, might work well in a Petri plate for projection too.

There are times when the authors may sacrifice simplicity in favor of the unusual. The various clock and oscillating reactions are not easily assembled or easily understood, but chemists everywhere will surely forgive such excursions from the basic text.

Some demonstration lecturers may want to quibble about the acetylene bubbles which replace the carbide cannon and the flame test of the fireworks elements that everyone does differently. The authors anticipate this and encourage the reader to modify the demonstrations to fit one's own needs.

It is a nice collection, clearly presented, with teaching tips and questions for students to consider following each demonstration.

James W. Cox, *The University of Montana*

Trace Analysis. Volume 4. Edited by James F. Lawrence (Food Research Division, Health Protection Branch, Health and Welfare Canada). Academic Press: Orlando, FL. 1985. xii + 305 pp. $65.00. ISBN 0-12-682104-6.

This fourth volume of the series continues the state-of-the-art, invited-expert(s) review format of the earlier volumes. Volumes 1 (1981) and 2 (1982) dealt largely with the application of high-performance liquid chromatography to organic and metal ion trace analysis in such diverse areas as water, mycotoxins, and vitamins, together with articles on detectors and enrichment techniques. Volume 3 (1984) expanded the scope of the methods to biological tissues and fluids, drugs, and environmental pollutants.

Volume 4 (1985) broadens the scope still further. L. Ebdon and B. A. King discuss the recent developments and applications concerning ion-selective polymeric membrane electrodes. Electrodes for ions include those for protons, sodium, potassium, lithium, calcium, magnesium, chloride, and nitrate. Ammonia and carbon dioxide electrodes are reviewed. Enzyme electrodes and biosensors are described for the measurement of urea, creatinine, amino acids, glucose, and nitrate. Drug detection electrodes, immunoelectrodes, and the measurement of mem-

*Unsigned book reviews are by the Book Review Editor.