Computer Software Reviews

NMR Simulator. By Paul Schatz, University Wisconsin, Milwaukee. COMPress, A Division of Wadsworth, Inc.: P.O. Box 102, Wentworth, NH 03282. List Price $95.00.

NMR Simulator is a teaching aid intended for training students in the operation of a Varian EM360 nuclear magnetic resonance (NMR) spectrometer. It is *not* a tutorial program and does not lead the student through a procedure in a controlled fashion. It does allow the student to investigate the effects of most of the spectrometer controls including radiofrequency power, coarse and fine spectrum amplitude, filter, sweep time, sweep width, sweep zero, integrator balance, and reset. The program does not simulate control over tuning via the phase, y, and curvature controls and this is unfortunate since it may lead to furthering the attitude that one merely "gets" the spectrum. The resultant spectrum may be plotted on a variety of output devices including dot-matrix printers such as the Epson FX, MX, and LQ series and plotters such as the IBM 7371 or 7372, HP 7470A or 7475A, or Sweet-P 100. The ability to control input directly via a mouse (Microsoft or Mouse Systems are supported) makes the exercise seem more realistic.

Features: The program requires a minimum of 256Kb of RAM, PC DOS (MS DOS) 2.0 or higher and at least one 360KB floppy disk. As supplied, the program includes two copies of the copy-protected 360KB program disk, a second sample spectra disk with 27 examples, and a manual describing installation procedures and usage. A library of 300 additional spectra is also available in groups of 75 spectra/floppy at $75.00 each or $250.00 for all 300 on four discs. The manual has separate sections covering mouse or keyboard controlled operation. The version provided to this reviewer was clearly defined as a preliminary version and did contain some serious errors. For example, upon completion of the installation procedure the user is advised to boot the system and type "MOCKNMR" to initiate the program. The correct initiation command for this installation was "NMR". The wrong command for control of the INTEGRATOR BALANCE was also provided in the section on Setting Up the Integral Spectrum. Nevertheless, it was possible to install the program and obtain several spectra within 2 h despite limited familiarity with the EM360 spectrometer. COMPress has also advised me that these errors have both been corrected in the current distribution versions of the program. Subsequent installation and demonstration to a colleague using his PC took less than 1 h. In addition to the stated IBM PC, XT, AT compatibility, the program was successfully run on an ATT 6300 with either monochrome graphics or ATT color graphics and on a Leading Edge system also with the Phoenix Bios. A TI-PC with 256K, hi-res monochrome graphics could not run the program. An extension of some interest is the ability to create transparencies showing the effect of individual controls by entering the GRAPHICS command prior to initiating the NMR Simulator. Subsequent use of ⟨Shift⟩ - ⟨Prt Sc⟩ permits dumping individual screens showing control settings and the corresponding spectrum. This reviewer would like to see the inclusion of an additional routine permitting users to create their own data sets for inclusion in the sample spectra. The program should prove useful in any environment where off-line training in the use of EM 3xx spectrometers series is needed or where training in the general aspects of CW ^{1}H NMR data processing is desirable.

William T. Winter, *Polytechnic University*

SURFER. Golden Software, Inc.: P.O. Box 281, Golden, Colorado 80402. Phone: (303) 279-1021. List Price $399 (academic discounts available).

SURFER is a scientific plotting package for IBM PC's, XT's, AT's, and compatibles. The outstanding feature of this program is its ability to create plots of functions of two variables (i.e., $z = z(x,y)$) as contour maps and hidden line 3-D surfaces, using a set of relatively sparse data points. The program can work with a regular grid of points established by other programs or can interpolate a regular grid from data provided for irregularly spaced points. SURFER also contains a two-dimensional plotting routine that plots x–y graphs, bar graphs, and pie charts. Overall, SURFER is user-friendly and versatile, with only a few drawbacks.

The program requires a minimum of 256 K RAM and DOS 2.0 or later. It can run on a double disk drive machine, but the program then resides on 3 floppies, which must be shuffled in and out. This becomes a nuisance; a hard disk eliminates this problem. The company suggests the use of an 8087/80287 math coprocessor to speed up gridding (that is, generating a regular grid from irregularly spaced points), plotting to the screen, and file optimization. The reviewers' machines have this chip; there was no problem with the speed creating a 25 × 25 grid with 47 data points. However, speed can become an important consideration. For example, creating a 100 × 100 grid from 400 data points with use of the relatively fast inverse distance interpolation option is reported to take 1 h on an AT equipped with the 80287 chip; the time falls to approximately 2 min to create a 25 × 25 grid for the same data. With an IBM PC (8088 based machine) without hard disk or math coprocessor, these times go up by a factor of 20.

The SURFER program contains sophisticated algorithms for interpolating a grid from an irregularly spaced set of data points. Methods to fill in the irregular grid and to smooth the resulting curves are available. The only practical limit to what can be done to make a contour or 3-D plot out of arbitrary data is that of calculation time.

A wide variety of printers and plotters is supported by this program: This list includes Epsons, IBM's, HP's, C.Itoh's, and Panasonics; check with the company for an updated list. If your PC is equipped with an IBM color or EGA board or Hercules graphics adapter, you can preview the graph you are creating and easily make changes before printing it out. Otherwise you can still run the program, but you must use the printout to develop the graph. The reviewers do not recommend this approach because of the time it takes to generate a printout. The contour graph generated by the tutorial, while of very good quality, took approximately 12 min to print out on a C.Itoh 1550 dot-matrix printer. Other printers and plotters may be significantly faster.

SURFER documentation is excellent, and the tutorial provided in the manual and accompanied by a data file on disk is a detailed step-by-step guide through the basics of this program. In addition, the company provides a toll-free number for technical support during normal working hours. The versatility of the program, easily accessed through its menu structure, is its real strength. For the surface plots, a variety of options exist: smoothing, hidden lines, changing angle of elevation and rotation, orthographic or perspective projections, and a variety of isoclines, point labelings, base filling, and axis displays. The x–y plotting routine allows plotting of multiple data sets with legends for each set. Various graphs can be stacked or set side-by-side on a page. SURFER comes with extensive symbol sets and fonts, including Greek and Cyrillic alphabets.

This program does what it purports to do, namely, it provides good surface plots and similar graphs on a small computer. The remaining question is, what will it be used for? We note that the program is somewhat slow for the complicated operations and that the speed will drop with the number of grid points. Three-dimensional plots are often the preferred method of presentation for data generated on a larger computer, which usually has provision for such plotting and would surely be much faster, although possibly not as versatile. On the other hand, simpler calculations and experimental data are often handled on a small computer and typically result in a requirement for plots generated from fewer, randomly placed points: for these the SURFER program is appropriate.

Elaine Chandler and H. L. Strauss, *University of California, Berkeley*

The Enhanced Graphics Toolkit. Version 2.0. Connell Scientific Graphics: 51 West Dayton Ave., 204A, Edmonds, WA 98020. List Price $195.

The Enhanced Graphics Toolkit by Connell Scientific Graphics is designed to help mitigate the pain of programing for the EGA graphics standard. Having just completed a port of C_Graph's molecular graphics package, ChemCad, to the EGA, I can testify to the frustration involved in writing a hardware interface for the EGA. Anyone who has tried to decrypt IBM's EGA technical documentation knows that at best it is time consuming and at worst it is time consuming and wrong. It is hard, then, to deny the need for products like the Enhanced Graphics Toolkit.

The toolkit is a set of routines that allow the programmer to access the EGA's various graphics functions from an application program. These functions include clearing the screen, drawing lines, polylines, polygons, reading and writing the EGA's registers (to set color values etc.), writing graphics characters, and defining fonts. Fill patterns and drawing logic can be set (for example, XOR can be used when drawing a line to create a "rubber band" line). Some of the more interesting features supported by the toolkit utilize the additional page of graphics memory that is available when the EGA card has 256K installed. This capability allows the application to write graphics information unseen and then display it. Double buffering, using the two pages of graphics

memory, greatly enhances the quality of animation. A split screen feature, supported by the EGA and the toolkit, allows portions of both graphics pages to be displayed and the pan feature allows images larger than 640X350 to be stored and panned across. Routines to create solid spheres, developed for the representation of molecules, are also included. The demo that accompanies the toolkit demonstrates these capabilities and is itself an excellent primer to the features of the EGA.

It is important to understand the difference between toolkits and the larger (and more expensive) graphics systems on the market. The Enhanced Graphic Toolkit basically handles the hardware interface between the application and the EGA. It is not a complete, device independent, graphics package which would handle coordinate systems, mapping, clipping, etc. Systems that have these features have advantages for large applications that will be ported often. However, they incorporate features that are unnecessary for many applications and worse are inevitably "blackboxes" in that the programmer will never see the source code. The Enhanced Graphics Toolkit, by contrast, comes complete with source code. These larger systems are also expensive, especially if the program is to be distributed. The price of the toolkit and distribution license (if needed) is quite reasonable by comparison.

A number of languages are supported by the toolkit. These include FORTRAN (Microsoft and Ryan-McFarland), C (Microsoft), Basic (Microsoft), Turbo Pascal, and Assembler. Although it would be very difficult for the Toolkit to support all brands of compilers, other common compilers should be supported. Various printer drivers can be purchased separately, priced between $35 and $50. Most notable of these are drivers for the HP Laserjet and Laserjet plus.

The documentation for the toolkit is somewhat sparse. As a reference manual for the knowledgable user, the documentation is adequate but there is too little general discussion and too few examples for beginners. Additional illustrations would be very helpful in making the documentation more accessible.

While there are a few surprising omissions in the functions supported by the Toolkit (most notably the lack of routines to draw circles and arcs), this is basically a very useful product. Especially pleasing is the inclusion of the source code (in assembly). This code can be very useful in learning about the EGA and allows the user to modify the Toolkit to his needs. For anyone planning to write an application for the EGA or just wishing to gain some insight into how the EGA works, I can highly recommend this product.

Daniel R. Kuhn, *CGraph Software, Inc.*

The Egg. Version 4.2. Peregrine Falcon Company: 2330 Marinship Way, Suite 307, Sausalito, CA 94965. List price $495; multiple copy discounts available; chemistry library $125.

The Egg is a technical word processing program that supports both equation processing and chemical structure drawing. The minimum configuration necessary to run The Egg is an IBM PC or compatible under MS-DOS 2.0 or higher with at least 256K of memory, one 320K floppy disk drive, and either a color graphics card or a Hercules graphics card. An additional floppy disk drive or hard disk is desirable. The program will also run on PC compatible laptops provided that it has been installed on a 3.5 in. diskette. ChemLibrary is recommended if the capability of drawing chemical structures is desired. The Egg is copy protected; however, up to 3 copies can be made from the master disk.

The manual that accompanies The Egg is excellent for the novice user of word processors. A written tutorial is provided that anticipates the pitfalls that many first-time users will encounter. The occasional humorous comments are welcome breaks in the monotony of practicing simple applications. The Help! section is especially valuable. An investment of about 3 h of time is necessary to install and learn the basics of The Egg. Frequent use would be necessary to become truly proficient with the many features, since The Egg is not menu driven.

The word processor itself is not as flexible as products designed for text processing alone, such as Microsoft WORD. Users accustomed to these types of programs will find many functions clumsy. For example, when inserting characters into existing text, the line is not automatically reformatted to the previous margins. The paragraph or line must be manually readjusted. The lack of automatic word wrap is inconvenient when editing large blocks of text, but it can be an advantage when working with large equations or chemical structures. Another difficulty is the virtual inability to undo the previous command, which proves especially annoying to the new user. The Egg also does not automatically save all edits when you exit, nor does it prompt the user to do so. While The Egg does not provide an optimum environment for text processing, it is certainly a workable system.

The strength of The Egg is its equation editing capabilities. An extraordinarily large set of symbols is provided, including 5 sizes of integral signs and various type of brackets. The reference card indicating the location of the symbols on the keyboard would be easier to use if the standard alpha-numeric keyboard were superimposed on it. Additional symbols beyond those included with The Egg may be obtained by using a simple strike-over utility or can be designed by the user. Bold, italic, and different size fonts are easily accessible. Creating subscripts and superscripts is convenient and up to 16 levels of subscripts and superscripts can be obtained on a single line. The manual provides some useful suggestions on constructing complicated equations.

Chemical structure drawing with use of The Egg requires some practice. A number of basic structures are provided with the ChemLibrary software, and these are indexed by name and functionality in an appendix. Unfortunately, no inorganic structures are included. The limitations of the keyboard make it more cumbersome than mouse driven programs such as ChemDraw, but complicated structures that occur frequently can be defined as single function keys. The instructions for using the library of structures are clear and a tutorial is provided.

Only a limited number of printers can be used with The Egg, but the list includes printers in a variety of price ranges and a laser printer (the Apple LaserWriter). The program was tested with a printer not on the list (the IBM ProPrinter) and good results were still obtained with only one exception—the extra large font appears with a horizontal white stripe. The manual is also not particularly clear about how to get correspondence quality output with the Epson or IBM printers. Bonds in most chemical structures appear reasonably smooth. The manual notes that the output in high quality mode from some printers *might* be acceptable to some journals as camera-ready copy. However, output from a laser printer would certainly be acceptable.

In conclusion, The Egg is well-documented software that allows users to create and edit equations with little effort, though strict text processing is somewhat cumbersome. Structures can be added to one's repertoire with practice. Chemists with a need to embed both equations and structures in their text will find this a useful program for the price.

Michelle M. Francl, *Bryn Mawr College*

The Scientific Desk. C. Abaci, Inc.: 208 St. Mary's Street, Raleigh, NC. Price: $1200.00 per year for unlimited site license, $530 per year for single machine license, $840 for unsupported single machine license. A 20% educational discount is given. User support and upgrades are provided only for licensed copies of the system.

The Scientific Desk is a library of over 600 FORTRAN subroutines and 10 application programs for scientific data analysis. Versions of the system are available or are under development for the IBM PC/XT/AT, RT, Apple MacIntosh, IBM 370/43xx/30xx, and VAX systems. The IBM PC version with only a subset of the library was evaluated for this review. For use, a FORTRAN compiler is required and the type specified when the system is purchased. At present, C. Abaci supports the IBM Professional, Lahey, Microsoft and Ryan-McFarland compilers for IBM personal computers. When run on an IBM personal computer, the system requires a minimum of 512 K RAM to run the application programs. Memory requirements to use the library will be based on the compiler type. A color graphics adapter (CGA) is required for programs or subroutines that employ graphics. While not required, a hard disk is recommended.

The manual provided with the system is massive (480 pages) yet provides only minimal information on using the system (70 pages). The majority of the manual is devoted to references and listings of FORTRAN comment lines for each subroutine. What information that is made available is somewhat scattered and no index is provided. Extensive documentation, tutorials, and most of the information found in the manual can be obtained on-screen when running any of the application or tutorial programs.

The major function of the The Scientific Desk is to make available a large number of computational subroutines for inclusion in user-written FORTRAN programs. The subroutines are derived from some of the most recently published methods that are referenced. The general areas of analysis supported include the following: arithmetic, linear algebra, interpolation, solution of nonlinear equations, optimization, differentiation, integration, differential equations, integral transformations, data fitting, statistics, data handling, error analysis, and elementary and special functions of mathematical physics. While a wide range of functions are provided, it is difficult to locate a specific function as the naming system is not descriptive. For example, a fast fourier transform routine is named J1A21 where one for regression is L8CP.

The 10 application programs referred to as Problem Solvers require no programming though a FORTRAN compiler and a copy of BASICA are needed to run some of the programs. These programs cover the areas of approximation, eigensystem analysis, zeros of polynomials, random deviates, linear algebra, vector/matrix arithmetic, linear regression, differential equations solving, overdetermined system solving, data plotting and fitting, quadrature, and statistical analysis. With each program, the user is provided with a menu of options that is consistent

from one program to another. The menus themselves are difficult to read when function keys are defined as they are displayed in gray on white. In most cases entry of a keyword is required to perform a specific function (STOP, PLOT, ANALYSIS, etc.) to perform a specific function and the function keys are not used. Extensive documentation for each of the Problem Solvers can be displayed from the initial program menu. This is required prior to using any of the programs as no instructions for their use is included in the manual. Once the analysis portion of the program has been entered, the instructions are no longer available though. Each program will allow for data entry from disk or keyboard, and where appropriate, graphs can be displayed in CGA mode (640×200 monochrome). Graphs can also be produced on an Epson compatible printer though they are not of publication quality.

The Scientific Desk should not be considered a general scientific data analysis tool but rather a resource for FORTRAN programmers doing extensive numerical analysis. Individuals familiar with FORTRAN programming should find the library quite useful, especially the graphics functions. For chemists who desire a rapid and convenient form of data analysis, other commercial products such as Asystant (Macmillan Software) or TK! Solver (Universal Technical Systems) would be more useful. In comparison, the Problem Solvers are primitive and should actually be thought of as demonstrations of the subroutines available in the Scientific Desk library.

James K. Hardy, *The University of Akron*

SANDRA—Structure and Reference Analyzer Program for the Beilstein Handbook of Organic Chemistry. By Alexander J. Lawson. Spinger-Verlag: New York. List price $500.00 (950 DM).

Colleagues here and abroad talk of the bygone days of organic chemistry when everyone knew German and used the *Beilstein Handbook of Organic Chemistry* the way broken English is the language of chemists and the *CRC Handbook* is used today. Well there is hope for a comeback for the *Beilstein Handbook*, the premier source of evaluated data and information on organic chemicals. Besides the 5th edition and all subsequent editions being written in English, the hope lies in the recently released program SANDRA, which is the abbreviation for Structure and Reference Analyzer. The program is very simple to describe, and it takes only one sentence. One draws a structure in an IBM PC using a mouse and hits a key, and the program analyzes the structure and comes up with a set of pointers as to where the chemical would be located in the 340 or so volumes of the *Beilstein Handbook*.

The *Beilstein Handbook of Organic Chemistry*, covering the chemical literature from 1830 to 1979 (Basic Series plus Supplemental Series I–V), systematically orders organic compounds by the number of carbon atoms, degree of unsaturation, and substitution patterns. The system is hierarchical and thus produces a unique location for every organic compound. Analogues and homologues are brought together under the system, so such compounds can be easily found. While not a lost art, there are few chemists today who can quickly and easily find a chemical in *Beilstein* without previously knowing the compound's specific index system number, since a basic knowledge of organic chemistry and German chemical nomenclature are required. (The latter is needed because once you use the molecular formula index, you must be able to know the German nomenclature to pick out your compound from the list of possibilities all having the same molecular formula.) Thus we have a situation tailor made for a computer. This complex but well ordered and structured classification scheme, the *Beilstein* system, has been programmed into a computer algorithm by Dr. Sandy Lawson, the Managing Director of the 5th edition of the printed *Beilstein Handbook*.

SANDRA, which is copy protected, comes on one disk and is easily installed on an IBM PC (or equivalent). The program runs best on a hard disk, but it will run on a floppy disk system. The program requires 256K of memory, a Microsoft or equivalent mouse, an IBM EGA graphics board or equivalent (a Hercules board version is due out in late 1987), and DOS 2.0 or later. There is a 78-page manual, which is reasonable, and it has many examples (there are 49 figures), but some commands are not explained (e.g., alternate bond mode), the index is sparse, and there is no detailed example of going from the output of the program to the actual printed *Handbook* volumes and pages. The program costs $500 (high, but perhaps not so high compared to the cost of the printed volumes, which now run about $20 000 per year for the 17 or so Supplemental volumes published each year). Information is available from the publisher regarding volume discounts for multiple copies within an organization. The program, like the *Beilstein Handbooks* printed volumes, is distributed by Springer-Verlag (ISBN 3-540-140046-8).

The program operation is very simple. It takes about half an hour to learn the particular commands of this structure drawing program. (It would be nice if one day there was a standard structure drawing program for all programs for chemists.) The program allows for entering up to 70 non-hydrogen atoms, which seems sufficient for most all purposes. One can use stereochemistry, as well as isotopes, but these have little meaning since these similar compounds will give pointers to the same locations in the *Handbook*. Once finished the program takes 2–12 s to come up with the set of pointers. The time depends on the complexity of the structure and the type of computer used. I have used both XT and AT class machines, as well as molecules up to the 70-atom limit. The program has worked every time, and when I have looked up the results in the printed version, the program had indeed pointed me to the right place. Sometimes the pointers are fairly broad (30–40 pages) and sometimes just a few pages. It all depends on the class of compound being analyzed.

The example I have chosen to use in this review is a simple one, 2-pyridinecarboxylic acid (molecular formula $C_6H_5O_2N$; Chemical Abstracts Service Registry No. 98-98-6). The SANDRA program pointers produced by the program are the following—Haupt-pages, 34 to 51; System-Number, 3249-3251; degree of unsaturation, $2n - 7$; Carbon Number, 6; and Supplemental Volume E III/IV 22/1. I went to the library and found the compound starting on the very bottom of page 33 of the Main (Haupt) volume and continuing on through most of page 34. The system number on the page was 3249, and the degree of unsaturation was $C_nH_{2n-7}O_2N$. I then went to the Supplemental Volume 22 and found additional data on this compound on pages 303–304. On page 303 there were the references to the *Beilstein Supplements E I and E II*, where additional data could be found on pages 502 and 30, respectively. SANDRA does not provide the information on these Supplemental volumes. The reason is stated in the manual: "If the required compound was only described before 1930 the entry can always be found using the General Index (H-E II) (General register). For this reason, SANDRA does not give any specific references to the Series H-E-II in the (pointer) field. However, the volume number (e.g., 22 in this case of E III/IV 22/1) naturally also applies to the single volumes in the same series H to E II." Personally I would prefer the additional information in the pointer field, even if it may appear to be redundant, since I feel few people will read the manual to find this out.

In addition to this compound, I also entered the 3- and 4-substituted acid, 3-pyridinecarboxylic acid (nicotinic acid) and 4-pyridinecarboxylic acid (isonicotinic acid). The SANDRA output was exactly the same, as would be expected. The actual data for these compounds were readily found in the printed volumes. For nicotinic acid, the data were found on pages 38–39, and for isonicotinic acid, the data were found on pages 45–46. These are both within the range of pages 34–51. Finding the additional data on these two isomers was readily accomplished, as they both follow the first compound by a few pages in each of the Supplementary volumes.

The program should be of great value to working chemists and should be a required part of any organic chemistry course and chemical information course. Hopefully the vendor will find a way to provide copies of the program to universities and colleges for such teaching purposes. My son who is taking organic chemistry in college this year received a short tutorial on *Beilstein* from a lecturer who had not received the proper training and had made little use of this valuable resource. It was clear from this experience that my son would never consider *Beilstein* as a source of chemical knowledge. During his spring break I showed him SANDRA, and he said "This I can understand and use".

In summary the program performs well. It does what it says it will do. Its accuracy is good to excellent. Given the wide range of organic compounds, and the varying amounts of information and the differing number of derivatives for a given compound, it would be hard to ask for more from this program. What is needed, and expected to become available within a short period of time, is a template and a handy user guide. After learning how to use the SANDRA, one should have to turn to the manual only for reference. A Macintosh version is not expected soon, as the market for such a version is said to be limited.

Stephen R. Heller, *Agriculture Research Service*

Mac240. Version 1.34. By T. Mitchell and S. Solon. White Pine Software: 75 Route 101A, P.O. Box 1108, Amherst, NH 03031. $199.

Mac240 offers the owner of a Macintosh with at least 512K of memory full emulation of DEC VT125 and VT240 graphics terminals, Tektronix 4010/4014 terminals, and VT52, VT100, and VT220 text terminals. Two copies of the program are provided, neither of which is copy protected. There is a bootable master disk and a backup disk also containing Kermit communication software, from Columbia University.

The great strength of Mac240 is its emulation of the VT240 keyboard. The F6 through F20 keys can be accessed from the Function menu as well as the Help and Do keys. The Keypads menu provides the emulation for the arrow keys as well as the E1 through E6 keys (Find, Ins, Rem, etc.) for text processing. The use of the arrow keys from the menu is impractical since the mouse must be moved to the menu and then to the

particular key emulation each time one cursor space movement is desired. However, if an Apple Numeric Keypad, Assimilation Inc., Numeric Turbo, or Mac Plus key pad is attached to the Macintosh, then the arrows can be accessed directly, allowing the Mac to be used almost as readily as the VT240 itself. Only the E1 through E6 keys and the F keys need a menu for use. Since these are used less frequently, this is not a significant detriment.

It is possible to replace standard ASCII with a number of different national character sets (for the use with multilingual documents) and to define four choices of fonts, which may be manually assigned to one of two character code lengths or invoked by host software.

Two aspects of the Macintosh require significant alterations from the VT240 itself. Since the Mac screen is smaller and the entire screen is displayed at all times, all coordinates are scaled down by two-thirds. This scaling is only a problem for highly detailed graphics. The colors are simulated on the monochrome screen by different patterns, except with text for which this technique is not acceptable.

The documentation and instructions are satisfactory but the spiral binding on the manual makes it difficult to turn pages. Several appendices cover in detail ReGIS graphics as well as Tektronix 4010/4014 graphics, pin configurations, and VT240 control codes. If the user is familiar with the Mac, then less than an hour learning time should be necessary to master Mac240's essential features.

Text and graphics can be incorporated into Mac applications by copying a selected region onto the clipboard and then pasting into another document. However, without the aid of Switcher, this process is very tedious requiring the user to quit Mac240 and then open the other document each time a text or graphic needs to be converted, or the selection may be pasted into the scrapbook. There is no capability to automatically save a selection as a text, Macpaint, or Macdraw document. If Mac240 is exited, the communication link with the host is preserved should Mac240 be again opened. It is possible to completely copy a region as a picture or simply the non-Regis drawn text. The text can also be copied to the clipboard as a table compatible with Excell or Jazz. Printing of the entire screen or of a selected region can be accomplished. A bit map is printed without any options for high resolution available. The Auto Print option prints each line of text as the cursor moves off the line.

All modems are supported for communication. The parameters for communication (baud rate, parity, etc.) can be saved and associated with a name and/or a phone number such that when it is selected under the Dial menu, the parameters are automatically set and the phone number dialed. Data transfers may be affected by using Kermit or Xmodem, both of which employ error detection. Xmodem may be used with Macbinary which allows a Mac file to be transferred to another Mac with its proper icon. A stream of characters may be saved or sent, without error checking.

Mac240 has a particular chemical application because at this time there is only one other emulator (Tekalike) which will allow the Macintosh to interact with Macromodel (1.5), a powerful molecular modeling and graphics program available for Vax computers. Although the VT241 is not recommended by the Macromodel developers as the graphics terminal of choice, Mac240 does provide the Mac owner adequate access to Macromodel. However, several limitations in its use should be considered before Mac240 is purchased for the sole use with Macromodel. The size and lack of color of the screen make viewing large molecules difficult. The atoms of large molecules become virtually indistinguishable while the resolution of the Mac is sufficient for text. The results of calculations are easily read as well as all the option buttons. The monochrome screen negates the color feature of Macromodel which normally aids in distinguishing atom types. The slowness of graphics can make Macromodel use tedious. Running Mac240 on a Mac Plus with Macromodel on a microVax, updating the drawing of a decapeptide required 25 s and almost as much time for the updating of the screen in changing modes.

Mac240 does not always give a perfect emulation of the hardware, resulting in misplaced text or a jumbled screen. If Macromodel is restarted, the problem usually is corrected. The Mac cursor becomes small cross hairs and is used to indicate a position for the full screen cross hairs. An option is selected with the screen cross hairs appropriately positioned and the space bar hit while the help file is invoked with a question mark.

Unfortunately, once interacting with Macromodel, only the Print Screen, Print Selected, and the Copy Text or Table options are available and then only with difficulty. It is not possible to save the screen image of a molecule on the Mac itself. Macromodel constantly awaits input from the user via the cross hairs and hence the Mac cursor is inactivated making menu access impossible. It is possible, however, to trick Mac240 by positioning the cross hairs in a neutral area of the screen and then hitting the space bar while simultaneously clicking the mouse over the menu bar. While Macromodel is processing the input from the screen cursor, it momentarily returns the small cross hairs to the standard arrow cursor of the mouse.

Overall, Mac240 provides the Mac user with the only means to fully exploit the power of the Vax editing capabilities. Communications are efficiently accomplished and customized for differing applications. It provides limited capabilities for file transfers as well as screen printing and graphic or text transfer with the clipboard for use with other Macintosh applications. Macromodel can be accessed and is relatively efficient for the manipulation of small molecules but is not acceptable for large systems, lacking the size and speed.

John Pojman, *The University of Texas at Austin*

Visual Molecules: Version 1.00. Molecular Parameters: Version 1.00. Kern International, Inc.: 100 Weymouth St., Suite G1, Rockland, MA 02370. List prices $75.00 and $65.00, respectively.

Visual Molecules allows the user to generate graphical display of a structure from crystallographic data and to determine bond lengths and bond angles. A related program, Molecular Parameters, uses the same input file to produce tables of bond lengths and angles and to calculate dihedral angles and least-squares planes in a molecule. Both are BASIC programs and are available for IBM, Apple, or Z-100 type personal computers. The IBM PC versions were used by this reviewer. Visual Molecules requires DOS 2.0 or higher, 96 KB of memory, a color graphics adapter, and an Epson or IBM dot-matrix printer for output. The requirements for Molecular Parameters are similar although the program will run with DOS 1.1.

These programs are not intended to replace sophisticated mainframe software associated with crystallographic structure display. Rather, they provide the chemist with an easy mode of visualizing a structure from published unit cell parameters and coordinates. For either program, an input file is created, and the program allows the selection of subsets of the atoms for drawing of bonds and calculation of geometric parameters. Visual Molecules displays the structure on the screen as a ball-and-stick model or as a stick stereoview. Input of x,y,z rotation angles generates different views of the structure. Individual interatomic distances and angles can be determined, but not torsion angles. The graphical display and input data can be plotted on a dot-matrix printer. Molecular Parameters creates the same data input file or will use one already stored from Visual Molecules. The structure is not displayed, but tables of bond lengths and bond angles for all or subsets of atoms are calculated. For large structures these calculations are quite slow; several minutes are required for a molecule of 30 atoms. Molecular Parameters also calculates torsion angles for specified atoms, least-squares, planes for a set of atoms, and distances of atoms from planes.

One potential drawback of these programs is that some knowledge of crystallography may be required. The programs do not take into account space groups or symmetry elements. The user may have to generate coordinates for atoms of a molecule related to others by symmetry if they are not part of the crystal data set. Similarly, if there is more than one molecule per unit cell, the user must provide coordinates for atoms in all molecules in order to view unit cell packing. These problems, though, are unlikely to arise for most applications of the programs to structures of organic molecules.

A manual is provided with each program, and both programs are very easy to use. The programs were apparently written to be usable with microcomputers of limited memory and therefore run less efficiently than anticipated for today's PC's. Since the BASIC programs themselves are provided, their features can be readily modified or extended. Visual Molecules should find wide application among both academic and industrial chemists as an aid for low resolution but inexpensive graphical examination of crystal structures. Molecular Parameters will be of use to those who, in addition, require calculations of torsion angles and planes.

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