

Additions and Corrections

Structure of a 12-Vertex Arachno Carborane, σ - $(\eta^5\text{-C}_5\text{H}_5)\text{Co}$ - $(\eta^5\text{-C}_5\text{H}_4)^+-(\text{CH}_3)_4\text{C}_4\text{B}_8\text{H}_8^-$, an Analogue of $\text{B}_{12}\text{H}_{12}^{6-}$ and $\text{C}_2\text{B}_{10}\text{H}_{12}^{4-}$, Mechanisms of Carborane Fluxional Behavior and Metallocarborane Formation from the $(\text{CH}_3)_4\text{C}_4\text{B}_8\text{H}_8^{2-}$ Ion.
JOHN E. DAVIES* and EKK SINN^{1b}

The space group of the title compound given in the abstract of ref 2 is $R\bar{3}$ not $I\bar{1}$.

The crystal structure of the title compound has been described by Grimes et al.² as triclinic, space group $I\bar{1}$, $a = 8.047$ (3) Å, $b = 37.05$ (2) Å, $c = 21.551$ (9) Å, $\alpha = 90.04$ (6)°, $\beta = 97.13$ (8)°, $\gamma = 89.94$ (7)°, $V = 6375$ (3) Å³, $Z = 12$ (3 molecules/asymmetric unit). This structure, however, is actually rhombohedral, space group $R\bar{3}$, $a = 37.03$ (2) Å, $c = 8.047$ (3) Å, $V = 9557$ Å³, $Z = 18$ (1 molecule/asymmetric unit). The triclinic vectors $[1/2 -1/2 3/2]$, $[-1/2 -1/2 -3/2]$, and $[100]$ define the rhombohedral cell.

The original reflexion data ($F_o^2 > 3(F_c^2)$) were obtained from the authors, reindexed, and merged in the $R\bar{3}$ setting. This yielded a total of 2372 unique reflexions in space group $R\bar{3}$ with an associated merging R factor of 0.02. The structure was successfully re-refined with this data set in space group $R\bar{3}$ (program SHELX,³ full matrix least squares, two refinement blocks, anisotropic thermal parameters for non-hydrogen atoms, riding model

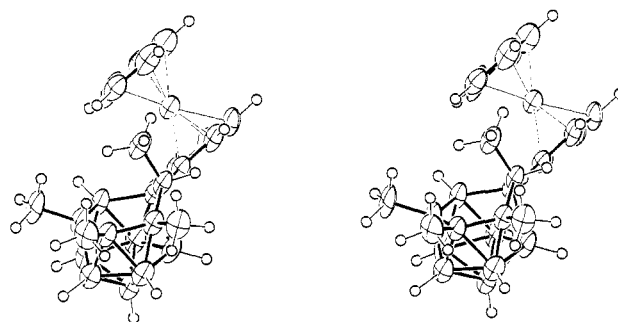


Figure 1.

for the hydrogen atoms), giving final values of $R = 0.049$, $R_w = 0.054$ ($R = \sum ||F_o| - |F_c|| / \sum |F_o|$ and $R_w = (\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2)^{1/2}$). Bond lengths and angles in the $R\bar{3}$ structure show no significant deviations from those reported for any of the three molecules in the asymmetric unit of the $I\bar{1}$ structure. Figure 1 is an ORTEP⁴ drawing of the $R\bar{3}$ molecule.

Supplementary Material Available: Tables of atomic coordinates, thermal parameters and bond lengths (8 pages); a listing of observed and calculated structure factors (14 pages). Ordering information is given on any current masthead page.

(1) (a) John E. Davies: Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, U.K. (b) Ekk Sinn: Department of Chemistry, University of Virginia, Charlottesville, Virginia 22901.

(2) Grimes, R. N.; Pipal, J. R.; Sinn, E. *J. Am. Chem. Soc.* **1979**, *101*, 4172.

(3) Sheldrick, G. M., 1976. SHELX76: Program for crystal structure determination, University of Cambridge, England.

(4) Johnson, C. K., 1965. ORTEP: Report ORNL-3794, Oak Ridge National Laboratory, Oak Ridge, TN.

Computer Software Reviews

VersaTerm-Pro. Version 1.00; 2/86. Developed by Lonnie R. Abelbeck. Distributed by Peripherals Computers & Supplies, Inc., 2457 Perkiomen Avenue, Mt. Penn, PA 19606. List price \$295.00.

VersaTerm-Pro is a terminal emulator for the Macintosh, emulating the Tektronix 4014 and 4105, DEC VT100, and the DG D200, providing access to both text and graphics applications.

It has several advantages over the terminals it emulates. Operating on the Macintosh enables it to incorporate output into the Mac environment as well as to transfer text prepared on the Mac to a mainframe. Output can be printed directly from the Mac on a variety of printers, including the LaserWriter, a capability which the emulated terminals lack. It also stores text in a buffer so that it is possible to scroll the screen in order to view a past interaction with the mainframe.

Operation of the program is easy to learn if the user is already familiar with the Macintosh pull-down menu format. The manual is very well done, covering all aspects in great detail with numerous examples. Incorporated in the **About VersaTerm-Pro** under the **open apple** is a help file covering all the major commands discussed in the manual.

Phone communications are facilitated by the ability to preprogram up to eight numbers which can be dialed from a pull-down menu. In addition, there is an **Auto Redial** feature that facilitates linking to heavily used phone networks. The system queries the user before disconnecting, making it virtually impossible to accidentally hang-up.

To speed login and execution of frequently used commands, up to ten separate string macros with 128 or fewer characters can be stored (under a label which need not be the same as the string itself) and executed from a pull-down menu. While each command normally executes a carriage return, this feature can be over-ridden.

VersaTerm-Pro exploits the mouse to its best advantage for text editing. On a VAX mainframe running the VMS, the mouse can be used to highlight text and copy it to the Mac clipboard. The information then can be pasted into the document at a different location or into a separate application.

An even more powerful capability is to use the **EMACS** mouse to control the cursor in the EDT edit mode. A file called "edtini.edt" must first be created defining the control characters which shift the cursor. When in the EDT text editor, there are two mouse cursors which can be used. The standard cursor is for highlighting and copying text. If the **Option** key is depressed, the cursor switches to **Edit Cursor**. (The **Show Edit Cursor** option may be selected for continual use of this feature.) When the **Edit Cursor** is pointed to a different location from the screen cursor, VersaTerm-Pro calculates and sends the necessary number and types of control commands to shift the screen cursor. This is a real time saver for users of mainframe screen editors. In EDT, the backspace key sends the cursor to the beginning of the line. With the **Map BS-Del** setting, the backspace key acts as a delete key as in regular Macintosh operations.

For users of the Unix operating system, two files entitled **termcap** and **terminfo** are included. These provide a description of the standard VT100 as well as the VT102 insert and delete character.

Since VersaTerm-Pro emulates Tektronix terminals, graphic output can be viewed, stored, and manipulated as a standard Macintosh document. Using the **Auto 'Tek 4014' Entry** option under **Extras**, the terminal emulation can be set to switch from VT100 (which is most suitable for standard text uses) to the Tek 4014 when a graphic output is received. A particularly elegant feature is the saving in memory of the VT100

screen while the emulation is in use, and vice versa. When a plot comes from the mainframe and the screen is switched to Tektronix emulation, the text screen which was operated upon is not lost. Switching back to the VT100 mode can be accomplished either by using the **emulation menu** or by simply pointing to the overlaid VT100 image.

Once the graphic output has been received, it can be saved. Note that it is not necessary to save the data to disk as it arrives, as in some other terminal emulators, but rather, at any time graphics can be saved either as Tekprint (as received) or as either a Macpaint or Macdraw document (neither of the latter two programs are included). A Macdraw document is created in a true Macdraw format with items created as objects. In the example tested, a plot with axes, labels, and a curve was saved as a Macdraw document. Each keyboard character was an independent object as were the axes and the curve. To move the entire curve, it was not necessary to first group all the pixels into an object. Graphics are scaled properly for the Macdraw format, but the text is not scaled relative to the graphics in order to obtain the best output. This feature can be overridden if the **scale text** option in the emulation Menu is checked.

Viewing of graphics is facilitated through the use of the **Zoom** feature which enables the user to enlarge an area of the screen. A rectangle can be defined by dragging the mouse cursor (a selection cross) while depressing the mouse button. Unless the shift key is held down first, the vertical dimension is adjusted to maintain the proper aspect ratio. Once a region has been selected, it can be enlarged to fill the entire screen with use of the **Zoom Selection** from the **Emulation Menu**. If **Zoom In** is chosen without first designating a region to be viewed, one-fourth of the screen, centered in the middle, is enlarged resulting in an image twice as large. **Zoom Out** reverses this process. **Revert to Top** sends the screen viewing back to default.

Versaterm-Pro supports the following printers: ImageWriter (RS-232) in which the ImageWriter is connected as an RS-232 device at 9600 baud, 8 data bits, and no parity (this provides the fastest output); ImageWriter (IW Driver) in which the ImageWriter is driven independently by the ImageWriter Resource software; LaserWriter (via Appletalk); Diablo 630 (RS-232), in which a Diablo letter quality printer is connected with the baud rate set in the **Baud Menu**; and Generic (RS-232) in which Versaterm-Pro does not perform any special printer control. This allows the mainframe to control the printing with the Mac serving only as a funnel for the data. Printing options available include **Print Stream** which prints text as it arrives from the mainframe, **Print Selection** which prints only the text on the screen to be highlighted by the mouse, and **Print Graphics**. When printing graphics, there is the option of a bitmap dump, which is a bit-by-bit reproduction of the screen, or of a full page printing that uses the maximum printer resolution. This latter option provides a very good reproduction of the graphic output without recourse to a plotter. The new version of the ImageWriter driver (2.1) is supplied with Versaterm-Pro. This driver supports single pass color printing with a color ribbon on the ImageWriter II.

The use of Molecular Mechanics calculations (Model) is facilitated by Versaterm-Pro with full screen cross-hairs on the Tektronix emulator. Using the Mouse makes molecule drawing simple. Each screen image can be saved and/or printed for documentation of the structures. Another use for any terminal for which Versaterm-Pro is especially well suited is accessing of data bases such as CAS Online. For example, the support of macro commands is a help for logging in when several codes are required. When a search is successful, the results can be printed directly with **Print Stream** or can be saved as a MacWrite document and later edited.

The transfer of files to and from a mainframe (without any protocol compatible programs) is accomplished with **Save Stream** and **Send Stream**. For communication with another Macintosh, **Mac XModem** is available. For CompuServe, then **TEXT XMODEM** is the standard file format. If an 8 bit data path to a mainframe is unavailable, then **Kermit** will do, requiring a 7 bit path for standard printable ASCII characters. It seems unfortunate that all the text documents must be saved and loaded from the Macwrite format. Users who prefer the superior formatting capabilities of Microsoft Word must transfer information first into Macwrite.

Difficulties may arise with this program and hard disk drives. MacDrive connects to the modem port, which is the preferred communications port. Normally, the printer is driven through the MacDrive from its port. Versaterm-Pro is compatible with this configuration except for high-resolution graphics. When High Resolution Graphics and the ImageWriter Driver were selected under the **Print Setup** menu and printing was attempted, the program locked and the system reset. **Print Steam** and bit-map dumping are still accessible. If a high-resolution picture of a screen image is desired, then the picture must be saved and printed by using the printer port after the modem has been disconnected.

Versaterm-Pro does not have any inherent chemical application but does provide access to several excellent terminals at a fraction of the cost, coupled with the ability to incorporate mainframe output into the Macintosh environment and exploit Macintosh abilities for inputting data.

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Fourier Perspective II. Produced by Alligator Transforms, Costa Mesa, CA. \$395.00.

FOURIER PERSPECTIVE II is a versatile package designed for use in work involving linear systems analysis.

FOURIER PERSPECTIVE II is distributed on four floppy disks and can be run on IBM PC, PC XT, PC AT, and most IBM compatibles operating under DOS version 2.0 or higher. Our work with this package was conducted on an IBM PC, an IBM PC XT, and an IBM PC AT. Most of the tests were done on the AT system; it includes an IBM Enhanced Graphics Adaptor (although not specifically referenced in the manual, all software ran on this also), 512 kB of memory, a 20 MB hard disk, and serial and parallel ports for plotter and printer, respectively. Although not required, an 8087 math coprocessor is strongly recommended to increase the speed of many of the more rigorous calculations possible with the package. Our system includes the 80287 coprocessor mounted on the Turbo 287 board from Microway, which speeds calculations even more than the 80287 alone.

To display the results on a CRT, an IBM color graphics board, Hercules board, or equivalent is required. Users should note that a Hercules board, as referred to in the Fourier Perspective II manual, is a Hercules Graphics card. Users with systems using a IBM Color Graphics Card or equivalent (a Hercules Color card was used for the test on the IBM PC-XT) should follow those instructions provided for IBM color graphics board users.

In order to obtain hard copies of results, a second package called Grafplus is recommended by Alligator Transforms. Grafplus is produced by Jewel Technologies in Seattle, Washington. This package is also distributed by Alligator Transforms. Grafplus is advertised to be compatible with several commonly utilized printers; however, this reviewer found his Olivetti printer not numbered among these. Grafplus was found unnecessary, and hard copy was obtained from an Olivetti PR2300 with the help of a short graphics routine included with the printer that configured the system to accept a Shift Prt-Sc command similar to that described in a discussion of Grafplus found in the FOURIER PERSPECTIVE II manual. Furthermore, users with IBM compatible printers (e.g., Okidata 192) will find that, when operating under DOS3.0, GRAPHICS.COM will serve as an effective substitute for Grafplus.

Operation of FOURIER PERSPECTIVE II requires a minimum of 256K RAM, but 512K RAM will allow utilization of the package's full potential. FOURIER PERSPECTIVE II requires two disk drives for operation, but in the presence of a hard disk, the system can be operated solely from this drive after loading. With copy protection being accomplished by means of a small nonmagnetic fingerprint on the system disk (disk I of IV), one duplication of this fingerprint region is made possible to allow use of the package as described above. If this fingerprint region is not duplicated on the hard disk, a system disk with its fingerprint intact must be present to initiate operation of the package. In either case, however, other files necessary to execute FOURIER PERSPECTIVE II can be backed up and run from anywhere. A word of caution is warranted in the event that those files are stored in a subdirectory of a hard disk. When such a method of backup is planned, it is important that the files be copied in the following fashion:

COPY d1:filename d2:/subdirectory/filename

If the files are copied as shown below

COPY d1:filename d2:/subdirectory filename

the filenames and the subdirectory name will be appended and this will render FOURIER PERSPECTIVE II unable to locate these copied files.

With the above exception, the procedures for loading and backing up FOURIER PERSPECTIVE II files are described in adequate detail and should present even the most inexperienced users with few difficulties.

Fourier Transform techniques are used by many professionals in a variety of fields that include everything from electrical engineering to chemical spectroscopy, and FOURIER PERSPECTIVE II provides a large variety of Fourier Techniques neatly packaged in an easy to learn menu driven format. While the package is not difficult to learn from an operational standpoint, the mathematics involved in many of the calculations would not be considered basic to those without previous exposure to the specific applications of Fourier techniques in their particular field of interest. Readers of the manual are frequently referred to an excellent monograph by R. Bracewell, entitled *The Fourier Transform and Its*

Applications.¹ The original work was published by McGraw-Hill in 1965, but a second edition was released in 1976, with an updated version of this edition having been released just this year. While mathematically correct and reasonably complete in its explanation of the various computations possible with FOURIER PERSPECTIVE II, these reviewers found the manual to be written with a bias toward workers in fields related to electrical engineering. Many of the terms used do not conform to those traditionally used in spectroscopic applications of the techniques discussed. In order to fully appreciate the detailed mathematics of the FT in spectroscopic applications, we would recommend Jansson's work entitled *Deconvolution With Applications in Spectroscopy*,² Griffiths' *Transform Technique in Chemistry*,³ and Marshall's *Fourier, Hadamard and Hilbert Transforms in Chemistry*⁴ for detailed introductions of the use of the FT in Chemical and Spectroscopic Applications.

The ability to read data from ASCII formatted files compiled with wordprocessing packages is one of the many powerful features of FOURIER PERSPECTIVE II. This feature was tested in our laboratory with WordStar and WorkMARC and found to be one of the most outstanding features of the package. For those to whom such packages are not available, the manual includes examples of BASIC programs that might be used to accomplish the same task. Furthermore, Lotus 1-2-3 user will be happy to learn that they can use their spread sheet data (.DIF files) as input for FOURIER PERSPECTIVE II.

Workers in our laboratory, with specific interest in the deconvolution of spectral data, have found FOURIER PERSPECTIVE II to be a tremendously efficient tool in exercises involving the choice of apodization functions for Fourier Self-Deconvolution and Fourier Filtering. Although only twelve predefined apodization functions are included with the package, the equivalent of apodization can be accomplished with the file manipulation commands. Similarly, while only two predefined filters are included (median window filter, and boxcar filter), other filters can be defined by the user who is willing to create BASIC ASCII files for them.

Several tools are also available to manipulate files; add two files, subtract two files, multiply two files, square a file, add a constant to a file, multiply a file by a constant, take the complex conjugate of a file, and multiply a file by its complex conjugate or the complex conjugate of another file.

In addition to those features already mentioned, FOURIER PERSPECTIVE II is capable of performing correlation and autocorrelation computations. All of these features and manipulations were tested in our laboratory, with both synthetic data files and real data from an FTIR. All features worked smoothly and clearly. However, it bears mention that, while the creators of FOURIER PERSPECTIVE II have taken great pains to develop a unique package that is easy to learn, extremely user friendly, and capable of executing complex computations at reasonably high speed, our major criticism of this fine piece of work is that it is of only limited use to most workers interested in the chemical applications of Fourier Techniques for linear systems analysis. Those willing to invest the effort necessary to modify the system by developing files for the apodization and filtering functions commonly used in specific applications like spectroscopy and electrochemistry would require an extensive and specific knowledge of particular mathematics prior to their introduction to FOURIER PERSPECTIVE II. This is not to say that such modifications are impossible, or even difficult; they are not. However, the creators of the package should expand the applicability of their product to an even broader scope by including apodization functions and filter functions commonly used by workers in other fields. Suggestions for apodization functions would include the sinc-squared, trapezoidal, triangular, Bessel, and Gaussian. Suggestions for filter functions would include Weiner-type smoothing filters.

In conclusion, Fourier Perspective II is not as chemically useful as it might be simply because it lacks some key manipulations with functions specific to chemical applications. This results in a package that is specific to electrical engineering applications. Although this is a good package for the general use of the FT in signal processing, for the chemist who is interested in a more global use of the FT with other techniques of signal processing and acquisition, many other general packages (e.g., ASYST) exist which include the FT along with many other capabilities.

(1) Bracewell, R., *The Fourier Transform and Its Applications*, 2nd ed.; McGraw-Hill: New York, 1978.

(2) Jansson, P. A., Ed. *Deconvolution with Applications in Spectroscopy*; Academic: Orlando, FL, 1984.

(3) Griffiths, P. R., Ed. *Transform Techniques in Chemistry*; Plenum: New York, 1978.

(4) Marshall, A. G., Ed. *Fourier, Hadamard and Hilbert Transforms in Chemistry*; Plenum: New York, 1982.

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TechWriter, Version 2.21, CMI Software: 1395 Main St., Waltham, MA. List price \$395.00; educational discounted price \$295.00; optional dictionary/speller \$50.00.

TechWriter is a full-featured scientific word processing program for the IBM PC. It has all of the features of a dedicated word processor, including mail-merge and macro key definitions. As a scientific word processor, it is very powerful. It can display and print the Greek alphabet and has all of the necessary technical symbols for the most demanding mathematics and physics equations. It also has all of the necessary "building blocks" to draw organic chemical symbols. The screen displays the text and the symbols as they will print out on a dot-matrix or laser-jet printer.

Features

The program requires a minimum of 256 Kb of RAM. Although it may be run with two floppy disk drives, a hard disk is recommended. The program may be run with the Enhanced Graphics Card, Color Graphics Card or the Hercules Monochrome Graphics Card. TechWriter is a WYSIWYG (pronounced Wizi-Wig: What-You-See-Is-What-You-Get) word processor. All fonts, standard or technical, are displayed on the screen as they will be printed out. The page is formatted on the screen as it will appear on the printed page. Formatting codes are normally hidden, but the user may reveal them for editing purposes. In order to accommodate all of the technical symbols and special functions associated with typing equations, the keyboard is totally "remapped" except for the main alphabet section. A template is provided for the standard IBM-PC keyboard and the IBM-AT keyboard. A variety of printers are compatible with TechWriter, including the "industry-standards" like Epson, Toshiba, NEC, IBM, Diablo, and the HP Laser Jet. The program is copy-protected but you are allowed to install it into your hard disk.

Performance

If you have used any other word processing programs for the IBM PC you will find TechWriter to be very slow. If you are used to some of the "speed-demons" like WORDPERFECT and XYWRITE you will find TechWriter to be absolutely intolerable. But to be fair, it is not slower than any other scientific word processing program for the IBM PC. The problem is that the technical fonts are not part of the hardware-based character set in the computer so the program has to create each character bit by bit (literally) on the screen as they are being displayed. In the case of TechWriter, regular characters as well as special characters are created by software. Thus, every time the screen is changed (page up, or down, inserting text in the middle of a sentence, etc.), the whole screen has to be redrawn bit by bit. On an IBM PC/XT it may take as long as 25 s to load a 2-p document and more than 5 s to scroll through each page on the screen. It does not take a very good typist to out-type the cursor. The manuals do make a point of reminding the user over and over again not to worry and assures the user that the computer will ultimately catch up. This snail-paced operation is particularly annoying when you invoke some functions which may cause the cursor to disappear for as long as 10 s while the program decides what to do next. The beginner may be left with the awful feeling that he/she has sent the computer to never-never-land and may type some other keys in desperation, thus compounding the problem. An example of this is setting up for boldfaced type. After you invoke the boldfaced type mode, the cursor will disappear for 5 s. If you are a confident typist, you can type ahead without any feedback on the screen. After the 5 s, a message appears on the top of the screen to tell you to type the "CONFIRM" key. After you hit the CONFIRM key, the cursor will again disappear for another 5 s while the text is being changed to appear boldfaced! The program was not tested on an IBM AT, but it is presumably faster.

TechWriter is both menu-driven and command-driven. When you first start the program (it takes a full 30 s to load the program!) you can select from a menu of operations; Create a New Document, Edit an Existing Document, Print a Document, etc. Some menus display sub-menus. Once you are in a document, all actions are command-driven by function keys on the keyboard. The document screen of TechWriter is very clean, with only a status line on the top which tells you what document you are editing and the mode you are in. Since the first 3 lines of the screen are reserved for prompts or error messages, you are left with only 20 lines for text. There is a curious presentation of the status line. The column, line, and page counters *do not* show the existing position of the cursor; rather, they show the position of the upper-left-hand corner of the text on the screen relative to the beginning of the document!

The appearance of the text on the screen rates from unacceptable to OK depending on the type of graphics adapter card you have. On a regular color graphics adapter card, the text is barely readable. Supercripts, subscripts, and scripted symbols like the Hamiltonian and Lagrangian are unrecognizable unless you know what you are looking for. On the Enhanced Graphics Adapter, the text is very much improved and is quite tolerable. For best screen appearance, the Hercules Monochrome

Graphics Card is recommended.

The program provides a large assortment of symbols, including the standard alphanumeric character set in both standard and scripted fonts, the complete upper- and lower-case Greek alphabet, and a bewildering collection of technical symbols for the mathematician and theoretical physicist. For the creation of organic structures, solid and broken lines inclined at multiples of 30° and at lengths that are multiples of half-spaces are provided. These are awkward to use and most unsatisfactory for anything other than draft purposes. Filled wedges, hashed wedges or lines, or curved lines are not available. There is a glossary and macro key feature which allows you to record key strokes for later use. If you spend the time to prerecord all your symbols, this feature will make the whole process of making chemical symbols a lot less painful. This version of TechWriter does not allow user-defined symbols. In August, 1986, CMI will release Version 3.0, which will allow the user to customize symbols (and presumably, organic structures).

In order to accommodate all of the Greek letters and technical symbols, the keyboard is totally remapped. Each of the regular alphabetic keys is used for eight different symbols. Functions are assigned to the F-keys on the left, the top-row number keys on the main keyboard section, and the numeric-cursor control keys on the right. The control and alternate keys (Ctrl and Alt) have identical functions and are used in conjunction with the other function keys to invoke more functions. The ESC key is the indent key, the INS key becomes the ESCAPE key, the DEL key is the HELP key, the "+" key is the CONFIRM key, etc. There seems to be no logic to the function key layout. Key F10 is Underline and Shift-F10 is for Insert/Over-write/Math selection. Function keys like Shift-F10 (labelled I/O/M) are used to switch among three functions in a round-robin fashion. For example, to switch from Overwrite Mode to the Insert Mode, you have to hit the key twice, once to go to Math mode and again to go from Math to Insert Mode. What all this means is that you cannot use this program without the keyboard template. The template that comes with the program has the key layout for the IBM PC keyboard on one side and the IBM AT keyboard on the other side. A template for the popular Keytronics 5151 is not available.

To use the Math symbols on the keyboard, you invoke the Math-Mode; to use the Greek Letters, you invoke the Greek mode. TechWriter provides a very convenient way to type in long and complicated equations. A portion of the screen can be mapped out and put in Equation Mode. Since the portion of the screen defined for equation is in half-lines, one can use the cursor-up and cursor-down keys to place superscripts or subscripts. In this way there is no limit to the number of levels of supers and subs for equations. The section of the screen defined as equation mode is protected from automatic page breaks so that equations are not split onto different pages when text is added or the page is reformatted.

Redefining the keyboard and writing to the screen directly bit-by-bit also means that many memory resident programs which "trap" certain keystrokes will not co-reside with TechWriter. We managed to get SIDEKICK to work but not POLYWINDOW. Any programs that interrupt the screen, such as screen-saver programs and alarm-clock programs, will halt the computer most ungracefully, requiring a complete cold start (power down and restart).

Printer support is very good. We tried an Epson FX-85 dot matrix printer, a Diablo ECS impact printer with a Scientific/Math print wheel, and an HP Laser-Jet printer with a "J-font" Math cartridge and a "B-font" Times-Roman Proportional cartridge.

For the Epson printer, TechWriter supplies a low- and high-resolution printer driver. To say that the printing is slow is an understatement. At low resolution, it took more than 5 min to print a page with only 3 lines of equations. We did not have the patience to repeat the test with the high-resolution printer driver. The output is quite presentable for a draft printer. All characters and special symbols are easily readable and recognizable; they all look much better in print than on the screen.

On the Diablo ECS, the print quality is superb but you will be limited to character fonts available on the 192 character ECS scientific print-wheel.

The HP Laser Jet provides the fastest output with maximum flexibility. With the J-font Math cartridge, almost all of the technical symbols are built-in, and printing is as fast as the Laser Jet can print, which is quite fast. The print-out looks like it came out of a very clean typewriter. With the Times-Roman Proportional cartridge, the technical symbols have to be downloaded to the printer first. The first page takes about 3 min but subsequent pages take less than 20 s. For the initial wait, you will be rewarded with publication-quality type face, comparable in quality to any text books from the printing press, for all characters and symbols.

Documentation and Ease of Learning

TechWriter comes with two 8 × 10 in. 3-ring binder manuals. One is a Reference Manual and the other is the Installation Guide and Tu-

torial. The reference manual is very complete. However, there is no index, which makes looking up random subjects quite impossible for all but the most experienced users. The installation guide is very well written; even a novice computer user can install this copy-protected program. The tutorial comes in two flavors, detailed, cook-book-style lessons and a "quick study" guide. Most graduate students who have had previous word-processing experience will probably do very well by just glancing through the quick study guide. Office secretaries have mastered this word processor by working through the detailed lessons. There is on-line help by pressing the HELP (Del) key.

Prompts and Error Messages on the screen are quite cryptic, but a detailed list of explanations for each error and prompt is available in the Appendix section of the manual.

Error Handling

For the most part, TechWriter is fool-proof. We tried but were unable to make it lock up or crash. The only exception is when running with a screen interrupt program in the background. This fact is not mentioned anywhere in the manual. An automatic screen blanking program or pop-up alarm clocks will kill the program and requires a complete cold start.

The program is so fool-proof that you cannot exit without saving the document first. What this means is that if you mess up your existing version you will have to save it, then delete it, and then rename the backup version and call it back up. This seems like an unreasonable penalty for inevitable occasional foul-ups. The program does have a dangerous omission. If you select from the file management submenu to delete a file, you will be asked to type in the name of the file to delete. As soon as you type in the name and a carriage return, the file is gone. This is the first program we have encountered that does not give you a second chance or bring out a caution message like "Are you Sure? Answer Yes to Delete, No to ignore..."

The program does not support subdirectory path names for files. This is a severe limitation for research groups in which many students may be sharing this program on a hard disk. Every user's files will have to be dumped onto the same directory as the main program. Yes, you can be inventive and work around this by using the DOS "SUBST" command or you can buy one of the available FILEPATH utility programs.

Support

TechWriter comes in seven floppy diskettes, an installation disk, a system disk, a sample document disk, and four printer-driver disks. The program is copy-protected and you may install up to five copies. This makes the installation process much less of a nerve-wrecking experience than some of the other copy-protected programs like DBASE III which allows you only one copy. The program comes with a 90-day warranty, and if you send in the registration card, CMI will keep you informed of any updates to fix any undocumented features (commonly called "bugs") for a period of 6 months.

We called the technical support line six times (the technical support line is not toll free!) and all questions were answered promptly and correctly. Four out of the six times, we got the same person. She seems to know the program very thoroughly. This is one of the better tech-support lines we have used.

Value, Summary and User Reactions

At the educational discounted price of \$295, this is not an expensive technical word processing program, but whether you will have the patience to put up with its pokey operation depends on how badly you need to do technical typing on your IBM PC. Two copies of an earlier version of TechWriter (Version 2.0) have been used in the Berkeley Chemistry Department for about 18 months. One is used exclusively by an office secretary who migrated from an NBI dedicated technical word processor to the IBM PC. He sorely misses the NBI but has nevertheless mastered TechWriter using the tutorial and a few phone calls to CMI technical support. The other group installed their copy on an IBM PC/XT which is shared by all of the members of a research group. From the twenty or so graduate students using the program, the reactions were mixed. Those who have had no other previous word processing experience fell in love with the TechWriter; four 300-page long Ph.D. theses have been written with TechWriter in the last year and a half. Those who have used other word processors hated it; they would rather use WordPerfect or WordStar and leave blank lines to write in the equations later.

Overall, we rate the performance as marginally satisfactory with very good printed output, very good documentation (would have been excellent if there was an index section), ease in learning, excellent technical support, and good error handling. The speed—or more appropriately, lack of speed—is the main complaint. CMI has announced TechWriter Version 3.0, which may be purchased without copy-protection. This will allow the program to be executed from RAM-disk. The non-copy-pro-

ted version will cost \$150.00 more, but the improvement in performance may be worth it. In the meantime, programs such as Wordperfect, Microsoft Word, or WordStar are superior for straight wordprocessing. For chemical structures, MacDraw (*J. Am. Chem. Soc.* **1985**, 107, 6140) or the related program ChemDraw are vastly superior. The sole area where TechWriter may offer an advantage is writing that uses a lot of complicated mathematical equations; in these applications, TechWriter's lack of speed may be tolerable.

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Molecular Graphics on the IBM PC Microcomputer. Enhanced Version 2.0. By J. G. Henkel and F. H. Clarke. Academic Press: New York. \$129.50.

"Molecular Graphics on the IBM PC Microcomputer" is a program designed to draw and manipulate molecules in three-dimensional space. Although this program is designed for the IBM PC, a companion package is available from Academic Press for the Apple. The operation of the program requires access to proprietary IBM files which must be copied from the operating system diskette (DOS 1.1, 2.0, or 3.0) before the system will function. The program, which allows for the creation of a working diskette as a backup and does not strongly admonish against copying, is available at a list price of \$129.50 from Academic Press. This software is a scaled-down version of visualization and orientation programs which are available at much greater expense from a number of sources.

This program allows one to determine conformation and to organize molecules, for example, in crystal lattices or in enzyme pockets. It will accommodate systems as large as 1199 atoms and bonds. Its input geometry requires Cartesian coordinates as raw data and allows the user to establish connectivity. From the input structure it is easily possible to calculate bond and torsional angles, to enter atomic distances, to scale to internal coordinate systems, to zoom size presentation, to highlight one

structure in the presence of others, or to emphasize one atom or group of atoms in a molecule. It is possible to use the program to invert coordinates or to move molecules or parts of molecules in either rotational or translational modes. The program's greatest strength is in allowing two molecules to be superimposed, so that chemists can examine "fit" into macromolecular arrays. The program allows screen display enhancement with molecules portrayed as balls and sticks, as interconnected lines, or as space-filling atoms.

The major limitation of the program is its quite tedious requirement for data entry. The practicing chemist must have available Cartesian coordinates, either calculated from standard bond distances or as available from X-ray structure data. Such coordinates could also be obtained from either molecular mechanics for semiempirical calculations, and the program does allow for the use of auxiliary programs, e.g., the "space tablet", for direct input of drawn molecules. The string of commands used in the program is sometimes cryptic, although the authors do provide a help command which lists available commands as well as their interpretation. The accompanying manual is straightforward and easy to use. The program also has a good series of prompt messages when input or size exceeds program capabilities.

The program is not intended to replace physical molecular models, and the difficulty of entering data will undoubtedly make this application unwieldy for simply constructed molecules. In studies in which intermolecular interactions of large similar systems are of interest and in which input parameters need not be started from scratch but can be used to manipulate an existing structure on file, the program may find high utility. The images produced from screen dump onto a printer can also be useful as a graphic representation fit for public presentation. The manual is clear and well organized, so that nonexperts can easily use the package. In our opinion the software will be of great use to chemists required to perform "docking" operations as a method for study of intermolecular interactions and as a method for depiction of molecules in two dimensions.

Marye Anne Fox and David Shultz, *University of Texas*

Book Reviews*

Minerals and Rocks. Volume 18. Natural Zeolites. Edited by Glauco Gottardi and Ermanno Galli (Universita di Modena: Modena, Italy). Springer-Verlag: New York. 1985. xii + 409 pp. \$59.00. ISBN 0-387-13939-7.

This book is the first monograph devoted completely to the subject of natural zeolites. The treatise opens with a tutorial in the topology of tetrahedral frameworks observed in natural zeolites. By careful comparisons of framework topologies, the natural zeolites of known structure are categorized into six groups. The six chapters which follow are devoted to the history, crystallography, chemistry, and physicochemical properties of each naturally occurring zeolite, one chapter per framework category. The closing chapter provides data for several natural zeolites with unknown structure. These eight chapters are organized well and presented clearly. The text also provides two appendices containing X-ray powder patterns and some infrared spectra of the natural zeolites. The monograph includes many useful features such as excellent references and fine details, e.g., unit cell parameters accompany X-ray powder patterns. This comprehensive text on natural zeolites is an excellent reference for those working in the areas of mineralogy and zeolite science.

Mark E. Davis, *Virginia Polytechnic Institute and State University*

Drugs and the Human Body. Second Edition. By Ken Liska (San Diego Mesa College). Macmillan Publishing Company: New York. 1986. xiv + 386 pp. \$14.00. ISBN 0-02-371070-5.

Drug use and misuse are topics of intense public and medical interest. The term drug, defined broadly here as "any absorbed substance that changes or enhances any physical or psychological function in the body", covers a multitude of sins. This book examines the pharmacology and legal aspects of a variety of chemical substances ranging from relatively innocuous OTC preparations to the hardest narcotics and street drugs. Topics covered in depth include marijuana, the Pill, hallucinogens, tranquilizers, pain killers, and stimulants. There is also an extensive index, a glossary of technical and street terminology, and an appendix on structure/activity relationships.

If the book is written for "students with little or no background in science". In keeping with its intended use as a textbook for nonscience

students, each chapter begins with a check-off list of significant facts and concludes with a set of study questions. If style is somewhat condescending, the level of presentation seems appropriate for the target audience. Written in lay language, the book is eminently readable and is crammed with factual information on drugs and their effects. Although much of the material appears to have been taken from compendia such as the *Physicians's Desk Reference*, rarely is there a citation to the source of the information. This is unfortunate. The nonscientific reader, in particular, should be made aware that what we accept as fact is the product of basic research and has appeared in print in refereed journals or other technical publications. At the very least the author should have included a list of supplementary references for persons wishing to pursue a topic in greater detail.

It is the author's intention to provide objective information about drugs without passing judgement on their use. For the most part he succeeds, but on certain topics his tone becomes rather preachy. This is especially true in the chapters dealing with alcohol and caffeine consumption, in which his comments border on the evangelistic. On other occasions the author, a licensed pharmacist and college chemistry teacher, offers authoritative (albeit undocumented) medical opinions. His recommendations seem reasonable and prudent, but, in this era of litigation, medical advice should be left to the physician. Regardless, the reader would be well advised to heed the recurrent message of moderation and to take seriously the warnings of drug hazards.

Even a casual reading uncovered a number of chemical and typographical errors which should have been eliminated in this second edition. Chemical inaccuracies, such as the incorrect structural formula for pentothal sodium (p 346) or the synonymous use of the terms ethylene glycol and diethylene glycol (p 64) are excusable given the intended market. The typographical errors are merely an annoyance, but in at least one case (T. 12.2) the misprint was substantial. The net effect of the poor proofreading is to cheapen the work and ultimately to damage its credibility. Despite its imperfections, this is an interesting, informative, and often entertaining book. The level of scientific discourse may not be the highest, but the subject matter is timely, and the data are up to date. The book would make a fine text for a science course for nonmajors or could serve as a useful supplement to an elective upper-division chemistry course. Its merits outweigh its shortcomings.

Mark R. DeCamp, *University of Michigan—Dearborn*

*Unsigned book reviews are by the Book Review Editor.