Computer Software Reviews

Bookpro Plus. Version 4.0. Arisoft Systems: 25824 Dundee Rd., Huntington Woods, MI 48070. List price $295.00.

Bookpro Plus is a file/text manager for the IBM PC, XT, AT, and PS/2. The program is designed to allow the storage of references, research notes, etc., which can then be retrieved by performing boolean operator searches. The retrieved information can be reformatted in a variety of ways to produce reports and bibliographies.

The program requires 384K RAM and PC or MS DOS V 2.0 or higher. The program can be run from either a hard drive or two floppies, although as with all data base systems the program will eventually operate better off a hard drive. The program is sold on two floppies (either $5^1/_4$ or $3^1/_2$), with the program files on one disk and utilities and sample data base on the other. The program supports a variety of dot matrix printers, as well as the HP laser series. Bookpro is compiled in Borland C and is not copy protected to allow for personal backup copies only.

Bookpro is operated via a combination of menus and control characters. The manual is presented in a logical and straightforward manner and includes a step-by-step tutorial. Online help is also provided, in the form of an alphabetized list of commands.

Entering references or text is straightforward. Fields do not have predefined lengths (an improvement over earlier versions of Bookpro), which allows for efficient use of disk space. The maximum record size is 65 000 characters, which provides sufficient room for most applications. Records can be entered manually or read in from ASCII text files. This feature allows direct downloading from online data bases such as Dialog and ISI. Data from previous versions of Bookpro can also be updated to run on Version 4.0.

Bookpro allows for sophisticated boolean searches, using "and", "or", and "not" operators. Up to ten search keys can be used, and parenthetical nesting of operators is allowed. Searching the base can be done either globally (i.e., searching every field in every record for a given search string) or by searching a special file of indexed keywords, which are entered separately in each record. Two wildcard characters are also allowed, one representing a single character and the other an unlimited number of characters. Unfortunately, Bookpro does not allow restriction of the fields within a record to be searched. Numerical searches (i.e., records a–n) are also possible.

Bookpro includes two special features. The "browse" feature allows 20 records at a time to be displayed simultaneously on the screen. Unfortunately, the records cannot be wrapped around the as a result the user must keep scrolling the screen horizontally to view the entire record. This manoeuver is slow and annoying. Bookpro also allows creation and storage of up to 40 macros, a most useful feature that makes long, repetitive procedures much more palatable.

Printing capabilities are quite advanced and allow for the versatile generation of attractive reports. Features include the ability to specify formats (bold, underline, italic, etc.) for specific fields, allowing the direct preparation of bibliographies. The HP laser printer must be initialized manually each time a report is to be printed, which is cumbersome.

The major flaw of Bookpro is that the commands are often non-intuitive, and operation seems in some cases to be needelessly complicated, although some of these features arise from adopting the text editing command syntax of WordPerfect and WordStar. For example, search keys are entered with letter designations a–j. These keys are then related by boolean operators on a separate logic line. The logic operators are given the symbols "&" for "and", "," for "or", and "!" for "not". This leads to "logic lines" which look like (((c,(a&b))&e)&!i). Searching would have been much more attractive if the entire search statement could have been written out on a single line, without symbols for the operators.

Ultimately, the program fulfills its advertised features satisfactorily. Compared to similar database packages available for the storage of references, the search capabilities are quite advanced allowing for rapid retrieval of specific references from a large data base, without becoming impossible to use. Although the user requires some familiarization with the program to fully exploit its capabilities, chemists should find it quite useful for the maintenance of citation data bases.

Eric Toone, *Harvard University*

PCMODEL. Serena Software: P.O. Box 3076, Bloomington, IN 47402-3076. List price $495.00 (Academic price $200.00).

PCMODEL is a molecular mechanics program derived from W. C. Still's MODEL program as modified by Kosta Steliou. PCMODEL was adapted for the IBM PC by M. Mark Midland with further adaptations and incorporation of the MMX force field (derived from Allinger's MM2 and MMP1) by K. E. Gilbert and J. J. Gajewski. The program is designed to run on an IBM PC/XT/AT. It requires a graphics board, 8087/80287 math coprocessor, 640K of memory, and a mouse. This reviewer used two systems: an IBM XT with a graphics Edge monochrome graphics board and a Zenith 386 with a Z-449 video display board. The color helps in visualizing more complex structures, but one can get along nicely without it.

PCMODEL allows one to sketch a structure on the screen using a mouse, run an energy minimization using the PCMODEL force field, and print out a file with the optimized bond lengths and stretching energy; nonbonded distances and van der Waals energy; bond angles, bending and stretch-bend energies; dihedral angles, torsional energy; dipole interaction energy; and heat of formation and strain energy. To test the program we ran the following series: octane, 3,3-diethylpentane, *trans*-decalin, bicyclo[2.2.2]octane, adamantane, diamantane, cubane, isopropyl *tert*-butyl ether, 3,3-dimethyl-2-pentanone, and bicyclo[3.2.1]octan-3-one. The calculated heats of formation were in reasonable agreement with the literature (standard deviation 2.55 kcal/mol). In a second series, the heats of formation for norbornane, norbornene, norbornadiene, nortricyclene, and quadricyclene were calculated. The agreement with the literature was excellent, with the exception of quadricyclene, which was 13.9 kcal/mol too high. The chair form of thiacyclohexane was calculated to be 5.25 kcal/mol more stable than the twist boat form, which one can compare with an experimental estimate (4.02 kcal/mol: Burkert, U.; Allinger, N. L. *Molecular Mechanics*; ACS Monograph 177; American Chemical Society: Washington, DC, 1982; p 236). PCMODEL also allows calculations to be carried out on carbocations, radicals and carbanions. Calculations on radical intermediates were tested by calculating the difference in strain energy for parent polycyclic hydrocarbon and bridgehead radical for bicyclo[2.2.2]octane, bicyclo[3.3.1]nonane, adamantane, and homoadamantane. Using the data of Koch and Gleicher (*J. Am. Chem. Soc.* **1971**, *93*, 1657) for the relative rates of bridgehead hydrogen abstraction by trichloromethyl, a correlation for the log of the relative rates of abstraction versus the increase of strain energy was obtained ($r = 0.95$). PCMODEL will treat unsaturated systems if they are not conjugated and organometallic systems; if conjugation is present, a program with a π atom calculation such as the MMX program must be used.

In general PCMODEL is easy to use and works very well. All the commands available in the structure input, display module, and minimization mode work as described. During a minimization, it is often a good idea to watch the change in molecular shape in order to spot false minima. For example, the program seems to want to place the carbon–hydrogen bond at a bridgehead position off at an angle so that all bonds project into one hemisphere. The atom move function (MOV-A) can be used to place the atom approximately in the correct spot and the program will then be back on course. A particular strength of PCMODEL is that it is set up to allow one to create files for use with MMX, MM2, MNDO, and MOPAC. If one is doing these calculations, the price of admission is worth it just to see up these files in a matter of minutes per file for medium size molecules.

Peter K. Freeman, *Oregon State University*

Math Type. Version 1.55. Design Science, Inc.: 6457-B East Pacific Coast Highway, Suite 392, Long Beach, CA 90803. List price $149.00. Not copy protected.

MathType is an exceptionally versatile mathematical equation editor for Apple Macintosh computers. It is intended to complement the many available word processing packages that can utilize PICT format material. Thus, it is very easy to transfer equations composed by MathType to word-processor documents by use of "Cut" and "Paste" commands. In addition, a two-way interface between the TEX typesetting language is provided. MathType can be installed as a desk accessory running under the Macintosh Finder system or can be run as an application under Switcher or MultiFinder. It is compatible with MacWrite, Microsoft Word, PageMaker, MacDraw, and many other software packages, according to its developer. For this review, compatibility with those, as well as with CricketGraph and CricketDraw, was verified. By a combination of templates and symbols, the program permits composition and display

$$\int_0^1 a(x)b(x)dx = \lim_{n\to\infty} \sup\ \psi_n(a,b) \qquad \sigma_x^2 = \frac{1}{n}\left\{\sum_{i=1}^{n} X_i^2 - n\bar{X}^2\right\}$$

$$A = \begin{bmatrix} \frac{abc}{b+c} & ab & ac \\ ba & \frac{abc}{c+a} & bc \\ ca & cb & \frac{abc}{a+b} \end{bmatrix} \qquad \sin^{-1}(x) = \int_0^x \frac{dt}{\sqrt{1-t^2}}$$

Figure 1. Examples of MathType equations, reproduced from LaserWriter output from a Microsoft Word document.

of virtually any desired mathematical expression of almost any complexity. Figure 1 contains four such examples, directly reproduced from MathType output, pasted into a Word document and printed using a LaserWriter. Equations may be optimized for either LaserWriter or ImageWriter output.

Other currently available commerical equation editors that are roughly equivalent in function to MathType are Expressionist (List price $79.95) and MacEqn (List price $44.95). Although both are somewhat less expensive than MathType, the latter is significantly more user-friendly and appears to be a superior value, when ease of use and overall versatility is considered.

Features: A minimum of 512 Kb of RAM is required. Although, as with most Macintosh software, it can be run with use of only a floppy disk drive, a hard disk is recommended. This is visually oriented program that can easily be mastered in an hour or two by anyone familiar with operation of a Macintosh computer. The user interface is comprised of a set of symbols (the Symbol Drawer) and a set of templates (the Template Drawer). The first contains approximately 80 special mathematical symbols, including all the commonly used Greek Symbols, which can be placed in equations by clicking on them. Equations are constructed by first selecting from among 60 or so templates, most of which include some symbols (e.g., integrals, fractions, product signs, summations, etc.) and various empty slots, and then filling in the slots with appropriate numbers, variables, and symbols. As the equations are constructed, they are continuously displayed and updated, as they will appear when printed out. A useful "Zoom" function allows display at double size to facilitate work with complex expressions. The program allows automatic assignment of any font installed in the Macintosh system to each of the various functions within equations (i.e., functions, variables, vectors, Greek functions, Greek variables, symbols) in any of five different styles (bold, italic, underline, outline, and shadow). Default choices are easily defined to suit individual user's needs and preferences and equally easily redefined temporarily. Similar flexibility is available in selection of typesizes and equation spacing. Documentation supplied with the program is adequate and well-written and is supplemented with an on-line tutorial, which is included on the disk with the program.

In short, MathType is an easily learned versatile tool that should be invaluable to anyone routinely using a Macintosh for preparation of scientific manuscripts. It is a well-designed high-quality software package and offers sufficient flexibility and ease of use that it should have wide appeal to chemists.

Charles L. Wilkins, *University of California, Riverside*

*Book Reviews**

Chemistry of the Natural Atmosphere. By Peter Warneck (Max-Planck-Institut fur Chemie). Academic Press: San Diego, CA. 1988. xiii + 757 pp. $85.00. ISBN 0-12-735630-4.

The *International Geophysics Series*, of which this is Volume 41, was started nearly 30 years ago and has maintained a high standard ever since. This volume is a comprehensive review of tropospheric and stratospheric atmospheric chemistry up to about 1985. The general tone of this volume is descriptive, with great emphasis placed on presenting observational data. The description of concepts is relatively abbreviated, but useful; enough detail is presented for a student to follow an argument, but the details of derivations are omitted.

The range of subjects covered in this review is extraordinary, but few subjects are covered with great depth, probably due to space limitations. Nonetheless, references to the literature are very extensive and thorough: the bibliography requires more than 80 pages and there appear to be nearly 2000 references.

The book opens with a discussion of the physical properties of the atmosphere and a qualitative discussion of atmospheric circulation. Photochemistry and kinetics are covered in a cursory fashion, but in sufficient detail for a rudimentary understanding of atmospheric reactions. The chemistry of the stratosphere is described in an excellent chapter that includes an historical survey and a very complete review of observational data on ozone and other trace species.

Three chapters are devoted to the complexities of tropospheric chemistry. The first of these chapters describes the fundamental chemical mechanisms and the second concentrates on ozone distribution, budgets, and general behavior. The third chapter is devoted to hydrocarbon oxidation mechanisms, which are very complex and are central to understanding photochemical smog. The chapters on the stratosphere and troposphere are augmented by appendixes that tabulate critically reviewed homogeneous rate constants that were current in 1985 (and are still nearly up to date).

The second half of the book describes several diverse topics, including nitrogen and sulfur chemistry. Other chapters include a detailed discussion of atmospheric aerosols (size distributions, production rates, mechanisms for formation, etc.) and clouds (cloud formation, scavenging of gases, chemical reactions in cloud droplets, etc.). The book concludes with two chapters on carbon dioxide geochemistry and atmospheric evolution. Each of these subjects is covered in some detail, with copious references to current literature.

In summary, the author achieves the two goals he has set for himself: "...to assemble and review observational data...and present concepts for interpretation ... in a manner suitable for classroom use." This collection of observational data is exceptional in extent and it will be an excellent source for atmospheric scientists. Concepts are presented in a manner most suitable for those who are already somewhat familiar with the field, but this volume could also serve as a text if it is supplemented in the classroom with more elementary material.

John R. Barker, *The University of Michigan*

Advances in Catalysis. Volume 35. Edited by D. D. Erley (The University Nottingham), Herman Pines (Northwestern University), and Paul B. Weisz (University of Pennsylvania). Academic Press, Inc.: London and Orlando. 1987. vii + 433 pp. $90.00. ISBN 0-12-007835-X.

This 35th volume of *Advances in Catalysis* continues in its tradition of providing comprehensive and informative reviews on topics of current interest in catalysis. The richness and diversity of research in the field is amply demonstrated by the variety of topics covered in the six chapters, spanning studies of single crystal catalysts, high surface-area supported catalysts, and phase-transfer catalysis.

The importance of structural studies has long been recognized as providing a foundation for understanding mechanistic aspects of catalysis. It seems appropriate then, that the extensive review (536 references) by Jan C. J. Bart and Gilberto Vlaic on extended X-ray absorption fine structure studies in catalysis be chosen as the first chapter of the book. The article is well organized; the introductory portions, which describe the experimental requirements and discuss the theoretical basis for X-ray absorption spectroscopy, are all written so as to be comprehensible to even a novice at EXAFS. The majority of the article deals with, as is advertised by the title, applications of EXAFS to catalysis with emphasis on supported metal and multimetal systems. Attention is focused on studies that characterize the identity and distance of nearest neighbors to the metal in the first few coordination spheres, and how these change with catalyst preparation, activation, and chemisorption on the surface. These structural properties are at times nicely compared with chemical properties such as reactivity and valence. A section on sulphided catalysts, currently of interest due to their relation to hydrodesulfurization reactions, concludes this important article.

The second chapter, by Daniel J. Driscoll, Kenneth D. Campbell, and Jack H. Lunsford, deals with the formation, detection, and role in catalysis of surface-generated gas-phase radicals. Both the method of detection and the reactions that generate the radicals are described in the review. Samplings are taken from studies utilizing mass spectrometry, matrix-isolation infrared spectroscopy, laser-induced fluorescence, matrix-isolation EPR, photoelectron spectroscopy, and resonance-enhanced

* Unsigned book reviews are by the Book Review Editor.