Computer Software Reviews

CHEOPS. Version 1.0. *CHE*mometrical *OP*timization by *S*implex. Elsevier Scientific Software: 52 Vanderbilt Avenue, New York, NY 10017. Attention J. Tagler. List Price $405.00.

CHEOPS is a suite of several programs useful for simplex optimization. Included in the package is a main driver, an input program which is utilized to define a simplex method (either modified or super modified), and programs to specify and name all the parameters needed (up to ten allowed).

CHEOPS is supplied on two floopy diskettes (object and source) and includes a user manual. Up to four copies of either diskette can be made under terms of the license. CHEOPS runs on the APPLE II family of computers (II, II+, IIe, and IIc) equipped with 48K (and a 16K language card), at least one diskette drive, and APPLE PASCAL (v1.1 or higher). APPLE PASCAL is not included as part of CHEOPS or the standard APPLE II package (i.e., not a part of DOS) and currently sells for $250.00 (Part No. A2W0016, v1.3). CHEOPS is also available for IBM-PC, XT, and AT microcomputers (128K, PC-DOS 2.0 or higher, 1 diskette drive, PASCAL). This review was conducted on the APPLE version of CHEOPS.

Installation is rather straightforward if you have a working knowledge of the APPLE PASCAL UCSD operating system (OS). The manual assumes the user has this background, and it only provides cursory help in both the installation (e.g., "use the FILER of the Pascal system") and operation (i.e., system related operations like file management). Since the majority of APPLE users will only be familiar with DOS, this could be a major stumbling block right from the start. A working diskette is created by copying the files from the first diskette to the APPLE PASCAL created blank diskette. The second diskette contains the PASCAL source code to the various programs (these are also listed in the manual), and as such they are not required for successful operation of the program. This code will allow modifications to be made to the existing code provided the user has a knowledge of PASCAL and the OS.

Although optimization methodology can be quite useful to a large number of chemists (e.g., analytical and large scale syntheses), the potential user hoping to learn these valuable techniques from this program will be quickly discouraged. The manual does provide a 24-page introduction to the subject, but I found it rather disorganized and quite sketchy. A brief bibliography is provided at the end of this section; however, the most recent application reference is to 1982. The remaining sections of the manual also provide rather terse coverage of their respective subject matter. Although default answers have been coded for most responses, the manual at best only provides a succint clue why these are preferred choices. Hopefully, the manual will be redesigned and improved for future releases.

On the bright side, the program does provide some helpful features. For example, the optimization procedure can be interrupted and saved for later reuse. This is a nice feature especially on the APPLE, when running large optimizations. The program is entirely menu driven, which also provides some necessary user-friendliness.

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Molecular Graphics (Molecular Graphics Program, Version 1.0). By B. H. Robinson. COMPress, Wadsworth, Inc.: P.O. Box 102, Wentworth, NH. List Price $500; educational discounted price $250.

The Molecular Graphics Program (MGP) is a "molecular display" program which is stated to run on the IBM PC, PC-XT, and PC-AT computers equipped with a minimum of IBM DOS 2.1-3.1, 512 Kb of memory, a Math Coprocessor (8087 or 80287), an EGA Card with 256 Kb of memory, and Enhanced Color Display. Mouse Hardware and Software is optional but recommended by the publisher. A 360 Kb disk drive is required for installation.

MGP was evaluated on an IBM PC-AT under DOS 3.1 with 640 Kb of RAM, a 30 Mb hard disk, an 80287 Math Coprocessor, an EVA/480 EGA Card, a NEC High Resolution Color Monitor, and a Microsoft Mouse. MGP and its accompanying files were copied onto the hard disk for use.

Three types of molecular representations of up to 600 atoms/work space (of which there are two) are offered, viz., wire-frame, shaded-ball with wire-frame, and shaded-ball with solid cylindrical bonds. Seven different colors are provided/ball and the ball size can be varied to give space filling representations. Specifically formatted files containing representations of some aromatic hydrocarbons, some cyclic and acyclic aliphatic hydrocarbons, some heterocyclic natural products, and some protein and peptide fragments are also provided.

To display a molecular representation by MGP, except for the examples accompanying the program, requires the user create (no Editor is specified and, presumably, any one is acceptable although only the Dewar Advanced Screen Editor Version 6.03 was used for this evaluation) a simple ASCII file containing the required information for that structure and, using a Fortran-like field identifier describing the data structure, to reformat the file with a special (provided) reformatting program. The data base for the file the user must create contains up to four pieces of information; a residue position number (for polymers, each unit is considered a residue; for nonpolymers, the entire group of atoms in a structure is considered a residue and no residue number is needed; however, the principle of using groups of residues, polymeric or not, can be a powerful and useful tool); a character label (for a system of a group of residues, e.g., polymers, the character label is one character in length and is used to identify the residue; for nonpolymers, the character label identifies a specific atom—H, C, N, O, P, S, other); three-dimensional Cartesian coordinates for each atom; and Bonding Coordination Numbers, currently limited to a maximum of four (which are automatically assigned on the basis of distances between atoms given by the Cartesian coordinates). An example of creating such a file is provided and, with a minimum of difficulty, new files can be generated—provided the Cartesian coordinates of the desired structure(s) are available. When such coorindates are available, only the tedium of data entry need be confronted and the annoying steps of reformatting the program, entry into MGP (a separate step) to see the structure and the necessity, in the event of error in data entry, of leaving MGP, accessing the unreformatted file, correcting the error, re-reformatting, and reentry into MGP to again see the structure. In this vein, and of considerable help, is the ability to unreformat, save as ASCII files, and examine the samples provided.

Once a structural representation has been created, its manipulation, in any of the forms provided, including (with a minimum of programming) loops for animation purposes, is easily accomplished with the lucid and logical command interpreter. The manipulation is facilitated by the Mouse menu and "docking of structures" or, indeed, even "molecular construction" through the use of previously defined fragments or residues is then possible. The resultant image can be stored. However, such "simple" procedures as ring inversion or molecular constructions (or "docking") involving, e.g., either rehybridization or inversion, will fail to give accurate representations (unless all necessary bond images are moved sequentially in small increments) since the originally defined geometries (excluding the single manipulation) are retained.

Within these limitations, one can readily introduce axes and rotate images globally or locally around them, highlight (or delete) portions of molecular representations, measure distances (but not angles), label nuclei, and search for specific interactions. Because of the use of the Fortran type format of the data file, this system lends itself to interfacing with other programs that calculate structural coordinates, such as Molecular Mechanics, and property formatted output files are easily reformatted with MGP for display.

The accompanying manual is generally well written and relatively free from error. The "HELP" commands are useful but are occasionally somewhat cryptic and simply reaffirm what the manual explains in detail. Regretably, there is no explicit provision for dumping the image produced to a printer/plotter.

Generally, MGP provides excellent graphics and routines for depicting structural representations. For cases where input parameters are available and with suitable programming, pictorial representations of a variety of useful transformations can be generated and manipulations of the representations, "docking" operations, and studies of "intermolecualr interactions" are easily carried out. Visualization of these operations might prove useful to both students and professionals.

David R. Dalton and Geoffrey R. Webster, Jr., *Temple University*

Bibliographer. Version 1.02. IRL Press Ltd.: P.O. Box 1, Eynsham, Oxford OX8 1JJ, U.K. No list price given.

The stated purpose of Bibliographer is to serve as a comprehensive database manager which enables the cataloguing, retrieving, and collating of bibliographic references; in other words it is a computerized card-file. Its features include the following: (i) cataloguing up to 65K references, each with 13 fields; (ii) retrieval by five different search routines, one of which allows the use of "and", "not", and "or" terms; (iii) preparation of reference lists formatted for publication and appendable to a word

processor; (iv) printing record cards for inclusion in a conventional card-filing system (for Luddites); and (v) full editing capability.

Bibliographer is written for the IBM PC equipped with at least 192K of memory and a DOS version 2.0 or higher. A color graphics card is not required. We have tested the program on an AT&T PC 6300 with 640K memory and DOS 3.1. With minimal effort, we were not able to boot the disk onto our departmental Northstar-Dimension which is frequently compatible with IBM software. The copy protection permits a total of three installations of Bibliographer to other floppies or hard drives. There is an "Uninstall" feature which permits the recovery and reuse of a copy.

The program is similar in intent to Notebook (Pro/Tem Software) and the Manager section of Sci-Mate, (*J. Am. Chem. Soc.* **1986**, *108*, 5042).

We found the input system for journal references highly structured with the following invariant fields: Authors, Title, Journal, Keywords, Year, Volume, Pages, Accession No., User No., Location, Marker 1, Marker 2, and Book. The author field requires a special format, i.e., Jones A.B., Smith C.D., White E.F., so that a special formatting routine must be used when references are collected to be transferred to a word processor if one wants a different author setup. There is also a special input framework for book entries. The benefit of this very structured input is that one-field searches for keywords, authors, etc., are very fast and easy to carry out. The minus side of the structure and indexing system is that a floppy can hold about 400–500 records (compared to Notebook 700–800 with similar formats). The complex search is very powerful, but probably not worth the trouble. A search table must be created which can have seven different fields, each searchable by either numerical, text, or logical criteria. This sort of powerful search algorithm might be useful when searching all of Chemical Abstracts or Beilstein but is "overkill" when one is dealing with a personal collection of 1–2K "cards". We find that single-term searches are the most easily and frequently used approach. One very nice feature of Bibliographer is "Browse" which is not a true search but a condensed display of all the records in alphabetical order or by accession number sequence, one screen at a time. A command permits the full display of any record spotted while browsing. From our survey of the program, the major deficiency is the technique for the extraction of a subset of references collected in a search. Each individual record must be marked as it is found and displayed, using a keyboard command. "Marker 1" must be activated to identify the record as part of a set which the operator wants to output to a word-processor while "Marker 2" must be activated to identify a subset which is to be saved as a separate file. This manual marking of sets of records is awkward (particularly when compared to Notebook). The conversion of records to ASCI text files does work. The records can then be incorporated into a word-processor. Printing of records without going through a word-processor is not easy, but it can be done. The required reformatting of the record so that the printed output matches the requirements of journal style is complicated enough to be annoying.

Overall, the software is fairly easy to learn and can be used by any chemist who needs to organize reprints, card-files etc.

Iris Anton and Richard W. Franck, *Hunter College/CUNY*

PC-ISP. Interactive Scientific Processor. Chapman and Hall: 29 West 35th Street, New York, NY 10001. List price $395.

PC-ISP is a command language for an IBM PC (with at least 640K RAM and two 360K floppys or one floppy and one hard disk drive) that can be used to analyze (e.g., statistically) experimental data. The language consists of about 74 commands and 72 built-in functions for operating on data sets of up to about 13 000 values. These include commands for manipulation of matrices, color graphic display of results, and curve fitting and smoothing. The commands can be clustered into short programs (macros) that can be retained as a file and used to carry out rather sophisticated calculations and data manipulations. The language is also useful in performing calculations, because a single ISP command can represent many lines of code in BASIC or FORTRAN. Thus only a few array-oriented ISP commands are needed to set up a series of numbers for a particular variable (x), calculate some function of x, and display the results by color graphics.

In addition to the many commands within ISP, such as "fft" to perform a fast Fourier transform or "smspline" that smooths data by constructing a spline function, a special command "cli" (command language interface) is available that executes an operating system command and returns to ISP. This is useful in editing ISP files and accessing FORTRAN and BASIC programs. The data files in ISP are read by an "input" command. This can be used to read the keyboard as well as both formatted and unformatted/binary files (e.g., produced by an A/D converter). ISP does not contain commands for data acquisition or external system control.

Full utilization of ISP requires a good familiarity with matrices and matrix operations and expertise in statistical methods. Thus to use commands like "stemleaf" (that does a stem-and-leaf display of data) or "polish" (that performs a median polish on a matrix table) you must know about Tukey's methods of data analysis. The documentation (a 234-page manual) is adequate for learning the ISP language, but it does not demonstrate or teach the basics of most of the statistical methods employed. We found that learning to use ISP involved a rather major commitment of time and effort. Since it is not a menu-driven system of packaged routines, it requires learning a completely new computer language that differs in syntax and structure from FORTRAN. For example, the MacIntosh program Cricket Graph was immediately used by workers in our laboratory to plot and fit data. This same group was largely unwilling, over a period of several months, to take the time to learn and use the considerably more powerful ISP system. There are several other useful systems for treating experimental data and doing calculations on the IBM PC. For example, the SAS software package that has been widely used on IBM mainframes is now available in a microcomputer version. It would probably be worthwhile for someone interested in one of these very useful packages to intercompare several in terms of scope, documentation, and ease of implementation before selecting one.

In conclusion, ISP is a new language and system that is useful for statistical treatment and presentation of data and for scientific calculation for those willing to make the non-negligible effort to learn the system and its fundamental capabilities.

Allen **J. Bard and Juhyoun Kwak,** *The University of Texas at Austin*

MacSpin. Version 1.1. D^2 Software: 3001 North Lamar Boulevard, Suite 110, Austin, Texas 78705. List price $99.95.

Here is a program that allows one to view complex numerical data from literally every angle. MacSpin is the first microcomputer implementation of sophisticated software for the graphical analysis of multivariate data in a way that was hitherto available only on mainframe computers. It runs on the Apple Macintosh (512K, 512K enhanced, or Mac+) and makes full use of this machine's graphical capabilities, as well as its user-friendly interface. Before describing what MacSpin can do, it should be stated that it is not intended for the display of molecular structures nor is it intended to replace spreadsheets or statistical analysis programs. It can be used very effectively to visualize the structure of complex data sets prior to carrying out full statistical analyses.

The program plots multivariate data, three variables at a time in three dimensions, allowing the user to rotate the data interactively around any of three perpendicular axes. In this way interesting features of the data, such as clustering, skewing, or the presence of outlying observations, can be quickly identified. Orientations which provide interesting viewpoints can be stored for future reference. In order to enhance the illusion of depth, the user may activate a feature that rocks the data back and forth a few degrees about a given axis. Specific data points may be identified by use of the mouse. In this way, the actual values of all the variables associated with a particular observation may be displayed right on the graph in a "pop-up menu". Extensive use is made of "pop-ups" throughout the program to make information instantly available as needed, without cluttering the display. In addition to individual observations, pop-ups providing numerical information pertaining to the current viewpoint, a particular variable, or a particular subset can be displayed.

The dependence of the displayed data on a fourth variable may be visualized by assigning it to the animation feature. The animation variable may be used to mask observations falling below (or above) a threshold value. Only those observations whose values of the animation variable fall above (or below) the threshold are displayed. The value of the threshold may be continuously varied by using on-screen controls, creating a "movie" showing the interaction of the fourth variable with the three that are displayed. The animation feature may also be used in a "slicing" mode.

It is impossible to describe all the features of MacSpin in a short review. The program allows one to create, select, combine and manipulate subsets of observations, to transform variables and create new ones with use of basic mathematical functions, and to identify observations falling within a certain range for a given variable.

Because the program conforms closely to the standard Macintosh user-interface, it is an intuitively easy program for an experienced Macintosh user to start using. Nonetheless, even the experienced Mac user should read the manual carefully in order to fully appreciate all of the features of the program and learn to use them effectively. The manual is complete and clearly written. A supplement is provided explaining the enhancements provided by Version 1.1. Those who have not previously used a Macintosh would be advised to first familiarize themselves by spending 1 or 2 h with the tutorial "A Guided Tour of Macintosh" that is provided by Apple with every machine.

The manual presents more than just how-to information; it is actually

a good introduction to modern concepts of graphical data analysis. The program comes with a second disk containing an extensive collection of real data sets taken from different fields. Important concepts underlying novel features of the program are illustrated in the manual by reference to these data sets.

When the Macintosh Clipboard is used, data may be exchanged between MacSpin and other programs, including Excel, Multiplan, Statview, Statworks, Cricket Graph, and the Data Desk. In this way, large data sets can be imported into the program without retyping. Graphical plots generated by the MacSpin itself may be copied and transferred via the Clipboard to MacPaint or MacDraw. The program works with the LaserWriter to create crisp hard-copy graphs.

One draw-back of the program is the difficulty of transforming variables except for simple formulas. The program lacks a parsing-capability that would allow the user to enter an arbitrary formula defining a ne variable in terms of existing ones.

This program should be useful to any chemist working with mult variate data. For example, it should be very useful to geochemists c atmospheric chemists studying the variation of chemical concentratior with height, depth, or distance. The program could also be useful t pharmacologists and biological chemists correlating structure–functio relations in a series of drugs.

The program's copy-protection scheme requires that the Master-dis be inserted every ten uses or every seven days. The program is availab from D^2 Software. To our knowledge no equivalent public domain c commercial software exists on any microcomputer.

Neocles B. Leontis and Deanne L. Snavely, *Bowling Gree State Universit*

Book Reviews

Thermodynamic Data for Biochemistry and Biotechnology. Edited by H. J. Hinz (Universitat Regensburg). Springer Verlag: Heidelberg and New York. 1986. XVI + 456 pp. $142.00. ISBN 0-387-16368-9.

The title of this treatise may imply that it is only a compilation of thermodynamic data. This is perhaps unfortunate. This book contains much more than tables of data. Each chapter is written by a recognized active worker in the field and is refereed by another outstanding contributor in the area covered by the chapter. Each chapter reviews the field concisely but adequately, providing appropriate introduction, theory and methodology, and tables of data with references. In most cases some interpretation of the data is included, with indications of important gaps in our current knowledge and areas that require further study.

The book is divided into six sections. Section I is an introduction by J. T. Edsall, including a brief and interesting history of the application of thermodynamics to biochemical processes followed by a discussion of the contributions of each of the chapters in the book.

Section II is entitled Nonreacting Systems and includes chapters by H. Høiland on Partial Molar Compressibilities, G. M. Mrevlishvili on Heat Capacities, and A. Cesaro on the Thermodynamics of Carbohydrate Monomers and Polymers.

Section III, on Interactions in Solution, includes chapters by H. Wiesinger and H. J. Hinz (Thermodynamics of Protein–Ligand Interaction), by P. D. Ross (Protein–Protein Association), and by B. G. Barisas (Hemoglobin).

Section IV is devoted to Solution Processes and includes Chapters by S. Cabani and P. Gianni on Gas–Liquid and Solid–Liquid Equilibria in Binary Aqueous Systems of Nonelectrolytes and by M. Luscher-Mattli on Biopolymer–Water Systems.

Section V deals with Phase Changes, including chapters on The Formation of Micelles by H. Hoffmann and W. Ulbricht, on Unfolding of Proteins by W. Pfeil, on Conformation Transitions in Polynucleotides by V. V. Filimonov, and on Oligonucleotide Transitions by K. J. Breslauer.

Section VI consists of a single chapter on Enzyme Catalyzed Processes by M. V. Rekharsky, G. L. Galchenko, A. M. Egorov, and I. V. Berenzin. This book provides an invaluable summary of available data and methodology in the fields covered by the chapters. The only negative comment deals with the, perhaps unavoidable, lead time required to produce a volume of this quality. The most recent references are at least 3 years old. Nevertheless, these chapters will provide a useful summary of available data, methods, and interpretation to the time of writing.

Siegfried Lindenbaum, *University of Kansas*

Advances in Organometallic Chemistry. Volume 25. Edited by F. G. A. Stone (University of Bristol) and R. West (University of Wisconsin, Madison). Academic Press: New York. 1986. vii + 399 pp. $79.50. ISBN 0-12-031125-9.

This volume contains eight fairly specialized reviews written by leaders in each field. The first chapter, "Silenes" by A. G. Brook and Kim M. Baines (44 pages, 209 references), outlines the preparation, physical properties, reactions, and molecular rearrangements of this interesting class of molecules. This tersely written review is quite comprehensive.

The second chapter, "Metalla-Derivatives of β-Diketones" by Charles M. Lukehart (36 pages, 57 references), covers developments in this field since an earlier 1981 review by the same author. The use of these complexes in metalla-β-ketoimine chemistry and in interligand carbon–carbon coupling reactions is emphasized.

"Organometallic Sonochemistry" by Kenneth S. Suslick (44 page 261 references) begins with a discussion of the physics of acoustic ca itation followed by a section on the devices used by chemists for ultrasoni irradiation. The limited amount of known sonochemistry of organ metallic complexes, both in homogeneous and heterogeneous systems, i described.

Chapter four is an informative review by Mark A. Gallop and Warre R. Roper on "Carbene and Carbyne Complexes of Ruthenium, Osmiu and Iridium" (77 pages, 138 references). The first section outlines rea sons why Fischer and Schrock type carbenes should not be viewed a separate classes of molecules. A detailed section on the bonding pro erties of carbyne ligands is also given. This is followed by an extensiv survey of the synthesis and reaction chemistry of carbene and carbyn complexes of these three metals. Particularly useful is the section o halocarbene complexes.

A comprehensive review entitled "Borabenzene Metal Complexes" b Gerhard E. Herberich and Holger Ohst (37 pages, 104 reference outlines the bonding characteristics of these ligands followed by th syntheses and reactions of their metal complexes. Similarities and di ferences of analogous cyclopentadienyl complexes are discussed.

The sixth chapter by Glen B. Deacon, Suellen J. Faulks, and Geoffre N. Pain is entitled "The Synthesis of Organometallics by Decarboxylatic Reactions" (39 pages, 169 references). The bulk of this article outlin in detail the preparation of both main group and transition-metal o ganometallic compounds by a variety of thermal decarboxylation rea tions. Many detailed examples are given.

Chapter seven is an informative introduction to "Detection of Tra sient Organometallic Species by Fast Time-Resolved IR Spectroscop by Martyn Poliakoff and Eric Weitz (39 pages, 112 references). It divided into three parts. The first section outlines general methods tha have been used to detect short-lived organometallic species. The secon section discusses the hardware, basically four different instruments, bein used to collect time-resolved IR data. Finally, the known experiment data are presented. This review is very recent, much of it coming fro the authors laboratories, including many 1985 publications and unpul lished results.

Finally, a comprehensive review, "Carbonyl Derivatives of Titaniun Zirconium and Hafnium" by David J. Sikora, David W. Macomber, an Marvin D. Rausch (62 pages, 117 references), discusses the preparatio properties, and reactivity (to form other complexes containing a carbon group) of this important class of compounds. The authors pay clo attention to detail, especially in the preparation section, frequently con paring and contrasting different preparative methods.

The topics in this volume are of interest to the organometallic con munity and it should be in every research library. Most of the topics a a little specialized to justify purchase for private collections.

Daniel L. Reger, *University of South Carolin*

Ab Initio Molecular Orbital Theory. By Warren Hehre (University California, Irvine), Leo Radom (Australian National University), Pa v. R. Schleyer (Universität Erlangen-Nürnberg), and John A. Pop (Carnegie-Mellon University). John Wiley and Sons: New York. 198 xviii + 548 pp. $79.95. ISBN 0-471-81241-2.

This book is not an introductory text in ab initio molecular orbit theory, though the first four short chapters do outline this theory an