ALCHEMY. Version 1.0. Tripos Associates Inc.: 6548 Clayton Road, St. Louis, Missouri 63117. (314) 647–1099. List price: $595 commerical; $350 academic.

ALCHEMY is a powerful desktop molecular modeling system designed for the IBM PC and MS-DOS compatibles. The elements of ALCHEMY are extracted from Tripos Associate's larger computer-aided molecular design software (i.e., SYBYL). ALCHEMY's major functions include the following: structure building, energy minimization, least-squares fitting of a series of molecules, and the generation of space-filling representations of molecules. The construction of a desired molecule is accomplished by hooking together molecular fragments in a manner analogous to a Drieding model. Energy minimization is via a molecular mechanics routine that uses analytical derivatives to find the local minimum. The molecular geometries of a series of structures can be visually compared by matching pairs of atoms with a least-squares fitting routine and viewing the superimposed structures. The overall shape of a structure can be viewed as a spacefilling model of the structure where the molecular surface is defined by its atomic van der Waals radii.

System Requirements: ALCHEMY requires an IBM PC, XT, AT, or compatible equipped with a minimum of 512 Kb of memory, one 1.2 Mb floppy disk drive or two 360 Kb floppy disk drives, one serial port, a mouse (Mouse Systems, Microsoft, or compatible) with software driver, an enhanced graphics adapter (or compatible) with 256 Kb of graphics memory, and an EGA monitor. Hardcopy of the molecular graphics requires a second serial port and a serial interface plotter which supports the HPGL-standard. A hard disk drive and/or a floating point (math) co-processor are strongly recommended. The program was evaluated on an IBM AT with an 80287 math co-processor, a 20 Mb hard disk drive, one 1.2 Mb floppy disk drive, one 360 Mb floppy disk drive, an IBM EGA card with enhanced color display, a Mouse Systems mouse, and a HP 7475A plotter.

Installation: The program is supplied on three floppy diskettes. Backup copies of the diskettes are made via the DOS diskcopy command. Diskette number 1 is a key disk (copy-protected) and gives an error during the copying process; however, the files are copied correctly. The program is installed on a hard disk drive by copying the contents of the diskettes into the appropriate subdirectory. For the program to run from the hard disk, the original ALCHEMY diskette #1 must be in one of the floppy disk drives. Once the program has started, diskette #1 can be removed and stored in a safe place. If diskette #1 is physically damaged, a replacement can be obtained from Tripos Associates for an unstated fee.

Before running ALCHEMY the first time, the configuration file ALCHEMY.CFG must be modified with an ASCII editor to indicate the type of mouse that will be used. Other options can be selected or changed within the program.

Features: ALCHEMY is a full-featured modelling package that is menu-driven and easy to learn. Commands are selected by moving the pointer to the desired "button" on the screen and clicking the mouse. The program is user-friendly with help available for the main menu and each sub-menu. The package is accompanied by a 122-page manual, which describes the display screens and all the commands. There is also a tutorial section in the manual that covers the basics of using ALCHEMY for molecular modelling. ALCHEMY can save and recall structures in SYBYL format, thus permitting ALCHEMY to exchange data with Tripos's larger modelling packages.

The molecular display options really distinguish ALCHEMY from other packages (see, for example: ChemCad review, *J. Am. Chem. Soc.* **1987**, *109*, 2229). Structures may be viewed in mono or stereo; the stereo view can be projected in either a relaxed or a crossed mode, and the stereo separation can be increased or decreased, as needed. In all display modes, ALCHEMY performs real-time translations and rotations; the screen updates are fast and provide smooth movement of the structure. The movements can be either global (affects all the molecules displayed) or relative (affects only the molecule selected). The direction and amount of movement (rotation or translation) is selected by positioning the cursor on the appropriate axis of an x–y grid in the lower right portion of the screen.

The display limitations of ALCHEMY are not stated in the manual; however, Tripos says the program can display ca. 1000 atoms with a comfortable viewing limit of approximately 300 atoms. Several molecules can be displayed at once, which is useful for manual or least-squares fitting. When viewing several molecules simultaneously, each molecule may be individually assigned one of 15 colors; the default setting colors each molecule by atom type (chemical element). ALCHEMY has a chiral/invert option that locates and assigns all chiral centers in a molecule. The chiral centers are assigned by the Cahn, Ingold, Prelog rules. Once the chiral centers are assigned, the molecule can be inverted (all the chiral centers are inverted) or a single chiral center can be inverted.

ALCHEMY optimizes the geometry of structures via a molecular mechanics procedure using analytical derivatives; the minimizer is derived from Tripos's larger mainframe packages. The size limitation of the minimization is not mentioned in the documentation; however, Tripos reports that molecules of ca. 130 atoms are the upper limit. We were able to optimize structures of ca. 150 atoms; experimention found that the upper limit is 200 atoms. The form of the equations used for minimization are clearly described in the manual. In addition, the manual provides clear instructions on how to modify the force field; the various parameters are stored in several files which are easily changed with an ASCII editor. Geometry optimization is rather fast with a math coprocessor (8087 or 80287) which is a recommended hardware option.

ALCHEMY also has the ability to compare two structures manually or via a least-squares fitting method. The least-squares method requires picking a minimum of three linearly independent sets of atoms from each molecule; the fitting process results in a root mean squared distance which is an indication of the quality of the fit.

ALCHEMY allows the user to access another program through an external command. This command temporarily halts execution of ALCHEMY, creates a file (EXTOUT.MOL) containing the coordinates of the current molecule, then executes the user supplied routine (which must be named EXTERN.EXE). When the external program has terminated, control returns to ALCHEMY which reads the molecular coordinates from EXTOUT.MOL, if it exists.

The molecular displays may be produced as hard copy by use of an HP-GL compatible plotter. The output may be a stick drawing analogous to the display on screen, or a space filled drawing where each atom is represented by a sphere with a radius equal to its van der Waals radius. The space filled drawing is a nice feature, but the plotting time is rather long.

Summary: In conclusion, ALCHEMY is a versatile desktop modelling package. The structure display options are diverse and useful. The real-time rotation (translation) of structures is fast and smooth, which permits viewing the structure from any perspective. Structure minimization for most molecules is reasonably fast for a microcomputer, especially with the suggested math coprocessor. The program interface is straightforward and easy to learn. The menu approach and on-screen help reduces the use of the manual. The space-fill display is nice, but very slow. The only output device supported is a plotter, since ALCHEMY is very color oriented. Support for other output devices (dot matrix printers, laser printers) would be nice since not everyone has access to a plotter.

George R. Newkome, *University of South Florida*

Book Reviews

Industrial Applications of Surfactants. Edited by D. R. Karsa (Lankro Chemicals Limited). The Royal Society of London: London. 1987. VIII + 352 pp. $65.00. ISBN 0-85186-666-2

The term surfactant has been identified in the past mostly with household cleaning and personal care applications. However, surfactants exhibit versatile characteristics due to their amphipathic behavior, which enables them to be employed in other than domestic usages. As the editor of *Industrial Applications of Surfactants* points out, approximately 40% of worldwide surfactant production is consumed in the industrial domain. This monograph highlights a diverse number of industrial applications which require surfactants. It is based on papers presented at an international conference held in April 1986.

Topics are divided into the following categories: main surfactant groups (Anionics, Cationics, and Nonionics), specific surfactant compounds (Copolymers, Fluorochemicals, and Silicones), and applications (Antifoams in Gas–Oil Separation, Antistatic/Conductivity Additives in Paints and Plastics, Coal–Water Slurries, Concrete Industry Applications, Emulsion Polymerization, Enhanced Oil Recovery, Fire Fighting

Foam, Industrial Hygiene Products, Mineral Processing, Organophilic Clays, Pesticide Concentrates, and Textile Processing).

Included in the overview of main surfactant groups is a discussion of structural types, physical properties, and applications. A valuable review of surfactant compounds which have been employed successfully in industry is provided in the introductory chapter. The author divides each general industrial area into specific subcategories and indicates those surfactants that are considered to be effective in each application.

Several chapters focus on the effect that a particular chemical functionality (Copolymer, Fluorochemical, and Silicone) has on surfactant performance. The Copolymer section should be quite useful to the reader because the author clearly illustrated the diverse characteristics obtained by adjusting the ratio of ethylene oxide to propylene oxide in the surfactant molecule.

Application chapters delve into the role surfactants serve to promote the completion of the industrial process. Two of the best sections deal with Fire Fighting Foams and Enhanced Oil Recovery. Both authors presented a detailed description of the processes and the evaluation procedures used to evaluate surfactant efficacy.

References are listed at the end of most chapters. The editor also contributed a subject index that is extremely useful to the reader. The only shortcoming to the book is that the editor should have paid closer attention to grouping relevant chapters together. In spite of the inconvenience, this book should be a valuable reference tool to those chemists involved with surfactants or the specific industrial areas mentioned.

Neil Canter, *Stepan Company*

Soviet Scientific Reviews. Section B. Chemistry Reviews. Volume 7. Edited by N. K. Kochetkov (Institute for Organic Chemistry) and M. E. Vol'pin (Institute for Organo-Element Compounds). Harwood Academic Publishers: New York. 1985. xi + 339 pp. $170.00. ISBN 3-7186-0154-0

This seventh volume in an annual series is the first to be devoted entirely to organic chemistry. The authors are presumably experts in their respective fields although their names are unfamiliar to this reviewer. Topics include tautomerism of azaphenylmethanes; reversible intramolecular migrations; metal-initiated reactions of alcohols, carbonyl compounds, and carboxylic acids; cationic reagents in electrophilic addition reactions; transition-metal-catalyzed diene oligomerization; and salt effects in electrophilic additions. The articles are written in uniformly correct English—they have been translated from the original Russian—and the quality of the typesetting and illustrations is adequate.

The preface states that this volume "reflects the achievements of Soviet scientists in various branches of organic chemistry". Accordingly, one might expect each of the six chapters to provide a survey in depth of a particular aspect of organic chemistry as practiced in the Soviet Union. This is not the case. Instead, the reviews are narrow in scope, simply summarizing results from the authors' own laboratories. At a price of $170, the reader is entitled to more thorough coverage.

One yardstick by which to measure review articles is the number of references to published materials. By this criterion there is a substantial variability in the quality of the chapters. For example, the section by Mamaev and Lapachev on azaphenylmethane tautomerism is very poorly annotated. Are we to conclude that the bulk of the chapter is based on unpublished data from their laboratory? On the other hand, the papers by Smit on electrophilic addition and by Tolstikov and Dzhemilev on diene oligomerization are extensively documented. The references, however, are not particularly timely; virtually all are to papers published prior to 1983. Curiously, throughout the book the majority of the citations are to papers or monographs published in the west. Perhaps this is an unintended commentary on the state of organic chemistry in the Soviet Union. Finally, if, as is claimed in the forward, the objective of this series is to make Soviet organic chemistry more accessible to western readers, it is unlikely to be realized. The purchase price will be prohibitive to all but the best endowed libraries. However, if there were interest in a particular subject, the economical alternative would be to order the individual chapter directly from the publisher at a cost of $30.

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

Synthesis of Macrocycles: The Design of Selective Complexing Agents. Progress in Macrocyclic Chemistry. Volume 3. Edited by R. M. Izatt and J. J. Christensen (Brigham Young University). John Wiley and Sons: New York. 1987. xi + 447 pp. $59.95. ISBN 0-471-82589-1

Since its inception the field of macrocyclic chemistry has been characterized by syntheses of novel compounds exhibiting unusual chemistry. A visionary goal of macrocyclic chemistry has long been to design complexes having specific reactivity with bound substrate molecules. This exciting volume of Progress in Macrocyclic Chemistry gives abundant examples of the diversity of approaches that have been made toward the accomplishment of this goal. Seven chapters by the leaders in macrocyclic synthesis are rich in the details of design principles, synthetic pathways, and selective properties of the resulting compounds. The stories of these molecules provide, in the words of one author, "an interesting mix of deliberate planning, persistant pursuit of goals, and serendipitous opportunism". In Chapter 1 complexes are described with exotic ligands providing the dual functionality of metal binding of dioxygen and noncovalent inclusion of an organic substrate molecule proximate to the metal center. The aim of Chapter 2 is to outline a rational method for the design of macrocyclic ligands for selective heavy-metal complexation. The subject of Chapter 3 is calixarenes, molecules known as "molecular baskets", potentially able to bind metal ions and substrate molecules in enzyme-like fashion. Chapter 4 concerns the design of cation and anion receptors, catalysts, and ion carriers. Chapter 5 contains a combination of experimental and theoretical studies of biological ion carriers that elucidates the factors determining ionophoric behavior. Chapter 6 returns to the theme of design and synthesis of ligands with the dual ability to complex both metal ions and organic substrates. Many exotic structures built from aromatic rings with multiple bridges result from a project to design molecular holes, niches, and clefts. The final chapter features synthesis and structures of inclusion compounds between macrocyclic ligands and uncharged organic molecules.

This book is an inspiring one. It leaves the reader not only with a sense of the impressive accomplishments in the field but also with a feeling of the tremendous potential for further development. The interdisciplinary nature of the subject and its applications should make the book useful to readers in all of the traditional areas of chemistry as well as those in interdisciplinary fields such as bioinorganic, organometallic, and medicinal chemistry.

Susan C. Jackels, *Wake Forest University*

Phosphorus-31 NMR Spectroscopy in Stereochemical Analysis. Organic Compounds and Metal Complexes. Methods in Stereochemical Analysis. Volume 8. Edited by J. G Verkade and L. D. Quin. VCH Publishers: Deerfield Beach, FL. 1987. xvi + 717 pp. $125.00. ISBN 0-89573-149-5

Phosphorus-31 NMR spectroscopy is a vital experimental technique in many areas, spanning organic chemistry, coordination and organometallic compounds, and biochemistry. For this reason, and the fact that the last major review of the field [Crutchfield, M. M.; Dungan, C. H.; Letcher, J. H.; Mark, V.; Van Wazer, J. R. In *Topics in Phosphorus Chemistry*; Grayson, M., Griffiths, E. J., Eds.; Wiley-Interscience: New York, 1967; Vol. 5] is now 20 years old, the new volume edited by Verkade and Quin is a very welcome and timely effort. Also, the coverage here is much broader than, and does not duplicate, that of another recent book [Gorenstein, D. G., Ed. *Phosphorus-31 NMR Princples and Applications*, Academic Press: New York, 1984] which deals mainly with the important biological applications of ^{31}P NMR spectroscopy.

This book consists of 20 chapters, written by recognized experts in their respective fields. More importantly, the editors have done an excellent job of planning and organization of the total subject. Readers new to the area are first introduced (Chapters 1 and 2) to the simple measurement and general interpretation of ^{31}P chemical shifts. These chapters also serve as a good outline for the detailed material that follows. The next several chapters (3–6) deal with experimental techniques (including 2-D and solid-state experiments) and theoretical considerations (both chemical shift and spin–spin coupling phenomena are well explained). Chapters 7–13 cover, in a logically progressive manner, particular applications of ^{31}P NMR to the solution of structural, conformational, and mechanistic problems in organophosphorus chemistry. The important concept of stereospecificity of ^{31}P couplings to all of the NMR-active nuclei is especially well treated in Chapters 11–13. The last seven chapters are devoted to all varieties of coordination compounds of phosphorus: unidentate, polydentate, bridging, one- and two-coordinate phosphines, ylides, phospholes, and phosphoranides. Although a great many types of compounds are covered, one noticeable omission from the book is the subject of poly(organophosphazenes). Given the technological importance of these P–N polymers, and the utility of ^{31}P NMR in their characterization, a chapter on such materials, and their cyclic analogues, would seem to have been warranted.

Overall, however, this is an excellent book with well-connected chapters that are remarkably consistent in terms of their level of coverage, clarity of organization, and comprehensiveness. Unquestionably, this is a landmark volume not only for the field of ^{31}P NMR spectroscopy but also for phosphorus chemistry in general.

Robert H. Neilson, *Texas Christian University*