Computer Software Reviews

Hyperchem. Distributed by Autodesk: 2320 Marinship Way, Sausalito, California 94965. List price: $3500.00; education discounted price $595.00.

Hyperchem is a molecular modeling program for the IBM PC or compatibles that was developed by Hypercube and is being distributed by Autodesk. Hyperchem requires Microsoft Windows, Version 3.0 and up, on an IBM 386- or 486-class computer with 4MB of RAM and 20MB of available hard disk space, an 80387 or 80487 math coprocessor, a VGA monitor, and a Microsoft or compatible mouse. Multiple copies of the program may be made, but a matching hardware key which connects to the parallel interface port is required. A version that runs on Silicon Graphics personal workstations, including the IRIS Indigo, has been released.

Hyperchem includes sophisticated molecular structure input and visualization which are interfaced with several molecular mechanics force field parameters: MM+, AMBER, OPLS, and BIO+, as well as the semiempirical methods CNDO, INDO, MINDO/3, MNDO, and AM1. Molecular dynamics simulations, as well as water solvation, can be performed. Manuals which cover the relevant background theory are thorough and well written, enabling one to quickly find the details of the calculational method being used. A Compuserve bulletin board has been set up, accessible by typing GO ASOFT.

Hyperchem was installed on our laboratory PC very quickly; the hardware key is easy to install, though regularly exchanging it between computers would not be convenient. The program is supplied with a few structures, including buckminsterfullerene and a set of amino acids, and one can rapidly access these structures. Further, the ability exists to read and write files in the Brookhaven Protein Data Bank format, and a few proteins are provided. Input and output of files in other formats, for example, SHELX, Cambridge, Brookhaven, and MDL files, would greatly enhance the ability to interface with other molecular structure programs. A short time with the manuals quickly explains the palatte of tools for drawing 2-D structures and converting these to 3-D structures which can be submitted for optimization. However, there are two minor shortcomings in the drawing tool: (1) the absence of an "undo" command and (2) the current element is not displayed.

We used Hyperchem to look at a range of organic and inorganic molecules as well as the supplied proteins. The MM^+ force field has been parametrized for the full periodic table, but the semiempirical methods have been limited to non-d-orbital elements with the exception of Si, P, S, and Cl. We found the system well suited for most biochemical and organic molecules, but inorganic molecules were handled less well. For example, modeling of the ferrocene molecule was limited by the ability to only have six bonding connections to a transition metal. Building, analyzing, and mutating polypeptides, on the other hand, was very well implemented. Building a polypeptide simply involves choosing the amino acids from a dialog box and, once built, the polypeptide can be viewed with the residues labeled. While Hyperchem is capable of handling up to 32 000 atoms, the time involved in any manipulation of large macromolecules can rapidly become excessive.

While it is possible to do molecular orbital calculations on rather large molecules, the time involved often becomes too great, especially when one is limited to an IBM PC. The solution that Hyperchem has offered is the ability to select a portion of the molecule of interest, create a Classical-quantum boundary, and do a molecular orbital calculation on the portion of interest. One can then plot electrostatic potential, total charge density, or molecular orbitals.

An exciting extension of the program is the ability to use Microsoft Excel or Microsoft Visual Basic to run multiple calculations and see the results of, for example, dihedral angle variation. This option does, however, require the user to purchase Excel 3.0 (earlier versions do not work).

For those who are considering an initial entry into the computing field and already possess an IBM PC with the requisite hardware, Hyperchem is an excellent choice. By including several force fields and easy modification thereof, the molecular mechanics alone is a step above PC-Model, and the addition of several semiempirical methods makes use of Hyperchem very exciting.

William R. Winchester and Michael P. Doyle, *Trinity University*

Book Reviews*

Coordination and Transport Properties of Macrocyclic Compounds in Solution. Studies in Physical and Theoretical Chemistry. Volume 76. By Brian Cox (ICI Fine Chemicals Manufacturing Organization, Manchester) and H. Schneider (Max-Planck-Institut fur Biophysikalische Chemie, Gottingen). Elsevier: Amsterdam and New York. 1992. xii + 418 pp. $164.00. ISBN 0-444-88613-3.

This monograph is rather broader than suggested by both the volume title and the series title. On the basis of the latter, one might expect to find a volume that is devoted to the physical chemistry of coordination and transport of cations by macrocycles. The authors themselves state that the "emphasis of this book lies in the fundamental aspects of the complexation reactions, with the major part being devoted to the thermodynamic and kinetic properties of simple complexation reactions, and of ion transport and extraction systems." Presumably because the above is emphasized, structural and synthetic aspects are mostly withheld until the end of the volume. Nevertheless, the presence of these facets nicely augments the volume making it deep in its principal focus while remaining reasonably broad in its coverage. The book's seven chapters are as follows: Introduction, Thermodynamics of complex formation, Kinetics and mechanism of complex formation, Solvent extraction of metal ions, Carrier mediated ion transport across membranes, Structural studies, and Synthesis of macrocyclic ligands.

The authors discuss cation binding and transport by macrocycles irrespective of whether the binders are naturally occurring or synthetic or are more applicable to alkali or transition metals or whether the principal donors are ether, carbonyl, or amine. Solution binding data obtained by a variety of methods are correlated to transport rates obtained by diverse methods. Transport in lipid and bulk organic membranes is discussed and correlated to binding and structure when possible or appropriate. In general, the discussion is thoughtful, insightful, and lucid.

A minor criticism is that a cursory survey of the references did not turn up any more recent than 1989. This is a little surprising as the volume has a 1992 publication date and was, according to the preface, prepared in camera-ready form. Although this is likely due to production time, one may argue that it is a problem for a book in a fast-moving field. On the other hand, this volume is primarily a review text and the principles discussed are well-referenced.

This monograph should be in the library of each practitioner of the macrocyclic art. Those peripherally involved in the macrocycle field, whether from the bioorganic, organic, inorganic, or physical subdisciplines, will find a wealth of understanding in this volume, but those new to the field may find it somewhat heavy going. It is a volume that nicely fulfills its somewhat specialized mission but offers a little extra that makes it a valuable addition to any library.

George W. Gokel, *University of Miami*

High Pressure Phase Behavior of Multicomponent Fluid Mixtures. By Richard J. Sadus (Swinburne Institute of Technology, Australia). Elsevier: Amsterdam and New York. 1992. xvi + 392 pp. $151.50. ISBN 0-444-88627-3.

In recent years much effort has been devoted to the investigation of multicomponent fluid mixtures at high pressures not only because of their extensive industrial applications, such as supercritical extraction and distillation processes and petroleum recovery, but also due to the development of new and more powerful experimental and theoretical tools for probing the microscopic as well as macroscopic behavior of these systems. The book compiles useful information on phase equilibria of ternary fluid (nonelectrolyte) mixtures via experiment and equations of state. The most important contribution, particular for practicing chemical engineers, physical chemists, and chemical physicists, is the presentation of numerous experimental results on phase behavior of several ternary systems and their correlation by simple equations of state and mixing rules.

The myriad varieties of thermodynamic and phase behavior displayed by fluid mixtures present a major challenge to the organizational concepts of classical and statistical thermodynamics. The observed equilibrium behavior of fluid mixtures can be classified in both molecular and ther-

*Unsigned book reviews are by the Book Review Editor.

modynamic terms. Molecular schemes classify mixtures according to the kinds of intermolecular forces acting among the constituent molecules (Rowlinson and Swinton, *Liquids and Liquid Mixtures*, 3rd ed., Butterworths, 1982, the reference of which is unfortunately missing from the book), while thermodynamic schemes focus on a progression in the behavior of particular macroscopic properties (Scott and van Konynenburg, *Discuss. Faraday Soc.* **1970**, *49* 87; *Phil. Trans.* **1980**, *A298*, 495) by dividing mixtures into different classes according to the behavior of mixture critical lines. This book focuses on the thermodynamic classification scheme of ternary molecular fluid mixtures in the space of different thermodynamic variables, such as temperature, pressure, composition, and volume, using results on high pressure phase diagrams obtained from equation of state approach and experiment.

The first three chapters of the book are devoted to a very brief survey of molecular scale computer simulations, basic thermodynamics of multicomponent phase equilibria, and various theoretical approaches, such as conformal solution theory, perturbation theory, and equation of state and mixing rules, while the latter part of the book (Chapters 4–9) deals specifically with high pressure phase behavior and critical phenomena of ternary molecular fluid mixtures. The latter presentation is nicely balanced between practice and theory, making the book easy to follow and a source of information that has genuine utility. Also included in an appendix are important experimental data on phase equilibrium of numerous ternary systems.

The book, though not suitable as a textbook, will be useful for a scientist seeking a guide to the literature on the high pressure phase behavior in fluid mixtures and will serve as a suitable reference book for those performing experiments at high pressures and intending to test their theories against experiment. However, the book lacks sufficient description of molecular approaches, probably because of the limited information available on rigorous theoretical methods (for example, computer simulation and statistical theory), to deal with phase behavior and critical phenomena in multicomponent fluid mixtures, but the list of recent references cited at the end of each chapter will largely benefit the readers.

Keshawa Shukla, *University of Houston*

Fortschritte der Chemie Organischer Naturstoffe/Progress in the Chemistry of Organic Natural Products. Volume 57. Edited by W. Herz, G. W. Kirby, W. Steglich, and Ch. Tamm. Springer-Verlag: Vienna and New York. 1991. x + 212 pp. DM 210. ISBN 3-211-82245-3.

The series of volumes initiated by Zechmeister, and colloquially known as "Fortschritte", continues to provide top quality reviews of pertinent areas of natural products chemistry. This volume is no exception, containing as it does three chapters on various aspects of the isolation, synthesis, biosynthesis, and biological properties of natural products. The high standards engendered by the previous volumes in the series are maintained in this volume, which is well-produced with very clear diagrams, complemented by a well-edited text, and two indices of authors and compounds and organisms. While this reviewer didn't find the former index very useful, the latter was especially comprehensive.

The first chapter by Metzger, Largeau, and Casadevall, entitled Lipids and Macromolecular Lipids of the Hydrocarbon-rich Microalga *Botryococcus braunii*. Chemical Structure and Biosynthesis. Geochemical and Biotechnological Importance, brings together the isolation and chemistry of the compounds, particularly the hydrocarbon and other lipid components, of the very interesting colonial green microalga *Botryococcus braunii*. Aspects of the biotechnology of this organism are also reviewed, since they directly relate to the potential development of a renewable source of hydrocarbons by a photosynthetic organism.

A review on the Carbazole Alkaloids is presented by Chakraborty and Roy in Chapter 2. It covers the structure elucidation, synthesis, biological activities, and chemistry of both the monomeric and dimeric alkaloids from the traditional source, higher plants, as well as the various groups of carbazole alkaloids isolated from the lower plants. The coverage is comprehensive and detailed, and the organization and content effectively show the importance of this class of alkaloids.

Finally, Pettit reviews The Bryostatins. These compounds, which were discovered by Pettit's group, are derived from the bryozoan *Bugula neritina* and have shown outstanding activity as anticancer agents. The chapter reviews the nature of the organism, the isolation of the bryostatins through bioactivity-guided fractionation, their structure elucidation, chemical transformations, and spectroscopic properties. There is ample discussion of the cytotoxic, antineoplastic and other biological properties of these important compounds. The chapter concludes with an overview of the potential of these compounds to be chemotherapeutic agents.

In summary, this volume continues the traditions of this excellent series and should be in every chemical science library and the personal libraries of many natural product chemists.

Geoffrey A. Cordell, *University of Illinois at Chicago*

Studies in Natural Products Chemistry. Volume 9. Structure and Chemistry (Part B). Edited by Atta-ur-Rahman (University of Karachi). Elsevier: Amsterdam, London, New York, and Tokyo. 1991. xvii + 632 pp. $220.50. ISBN 0-444-89165-X.

The latest addition to Professor Atta-ur-Rahman's continuing series of books surveying the chemistry of natural products is yet another cornucopia of chemistry. Its 24 chapters cover material as widely varied as X-ray crystallography, NMR spectroscopy, and mass spectrometry as structural tools, "bench-top" bioassay techniques, biosynthesis mechanisms, and descriptions of new natural products from microbes to higher plants. If there is a master plan to the overall organization of this series, it is at least as arcane as the enigma of Sir Edward Elgar's famous *Variations*. No one can accuse the editor of Germanic pedantry.

Almost without exception, each chapter has been written by an author or a group of authors who are currently active in their respective fields. The references are numerous and up-to-date. Chemists interested in the subjects covered by specific chapters will find this to be a very worthwhile source, and there is no doubt that the entire series of volumes is becoming an increasingly valuable reference work. Since it has become essentially impossible for an individual researcher to keep up with a field as large as this, the chances of discovering interesting and even useful research which would not have been otherwise encountered are good.

Some of the minor faults found in earlier volumes in this series persist. There are still almost as many typographic and formula styles as there are chapters. There is a subject index, but no author index, making it difficult for readers to determine quickly whether the seminal contributions from their own laboratories have been appropriately cited. Nevertheless, this volume demonstrates the enormous breadth and vigor of "natural products chemistry", and it represents a worthy contribution to the literature of one of the most vital areas of organic chemistry.

Jerrold Meinwald, *Cornell University*

Selective Reactions of Metal-Activated Molecules. Edited by H. Werner, A. G. Griesbeck, W. Adam, G. Bringmann, and W. Kiefer (Bayerische Julius-Maximilians-Universität Würzburg). Vieweg: Braunschweig/Wiesbaden. 1991. x + 236 pp. DM 98. ISBN 3-528-06450-1.

This book was developed from a symposium held in Würzberg, Germany, September 18–20, 1991. It contains, in typescript form, abstracts of 12 plenary lectures and 22 posters presented at the symposium. The posters are organized under the following headings: Project-Area A: Activation of dioxygen and C–H bonds in unsaturated molecules; Project-Area B: Development of organometal-assisted selective synthesis; and Project-Area C: Spectroscopic and theoretical studies on the structure and dynamics of metal-bonded molecules. There are no indexes, but the affiliations of authors are given at the headings of the lectures and posters.

Dynamics and Mechanisms of Photoinduced Electron Transfer and Related Phenomena. Edited by N. Mataga, T. Okada, and H. Masuhara (Osaka University). North Holland: Amsterdam. 1992. xviii + 568 pp. $148.50. ISBN 0-444-89191-9.

This book was developed from the Yamada Conference XXIX on the title subject held in Senri, Osaka, Japan, May 12–16, 1991. It contains a preface, a list of the organizing committee, a list of the participants, a welcome address by Syuzo Seki, a description of the Yamada Science Foundation, a list of the Executive Members of this Foundation, and 40 papers presented at the conference. These are organized under the following headings—Part 1: Fundamental Aspects of Electron Transfer and Related Processes. I; Part 2: Fundamental Aspects of Electron Transfer and Related Processes. II; Part 3: Electron and Energy Transfer in Molecular Aggregates and Polymers; and Part 4: Electron and Energy Transfer in Photosynthesis and Related Phenomena. There are indexes of authors and subjects.

Cluster Models for Surface and Bulk Phenomena. NATO ASI Series, Series B: Physics Volume 283. Edited by Gianfranco Pacchioni (Università di Milano), Paul S. Bagus (IBM Research Division, San Jose, CA), and Fulvio Parmigiani (Centro Informazioni Studi Esperienze, Milano). Plenum Press: New York and London. 1992. xvi + 694 pp. $139.50. ISBN 0-306-44102-0.

This book contains the Proceedings of a NATO Advanced Research Workshop on Cluster Models for Surface and Bulk Phenomena held in Erice, Sicily, Italy, April 19–26, 1991. It consists of a preface by the editors and 53 typescript chapters, which are grouped into the following catagories: Properties of Gas-Phase Clusters; Organometallic, Supported Clusters and Film Growth; Condensed Matter: Surface Processes; and Condensed Matter: Bulk Liquids and Solids. There are indexes of contributors and subjects.