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.

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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.

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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.