An in-depth understanding of how molecular modeling really works requires a prerequisite knowledge of molecular energetics at the level of undergraduate physical chemistry. At the graduate level, a comprehensive treatment of molecular quantum mechanics is available in such texts as Hehre et al.'s *ab initio Molecular Orbital Theory* (Wiley). Molecular simulation applied to chemical systems is effectively described in the advanced texts by Allen and Tildesly, *Computer Simulation of Liquids* (Oxford), and Haile, *Molecular Dynamics Simulation* (Wiley-Interscience), all frequently used in graduate seminars and for reference in research projects. Andrew Leach's book fits into curriculum between undergraduate physical chemistry and graduate level theory seminars, and serves as a complement to both. A lively and conversational style of writing and a good organization overall make this book useful and pleasurable for self-study as well. A unique feature is that each chapter is constructed to be as independent of the others as possible, which nicely facilitates "dipping in" as well as working through the book from cover to cover.

The authorial aim of the text is to provide (a) an introduction to the techniques used in molecular modeling, (b) theoretical background on the variety of methods available to the molecular modeler, (c) guidance in selecting the most appropriate method for a given problem, and (d) a practical description of the underlying theoretical principles. *Molecular Modeling* begins with a consideration of methods for computing molecular energies. One early chapter is devoted to an overview of molecular quantum mechanics and another to empirical potential functions. The level of presentation is geared to be more conceptual than mathematical, and practical rather than theoretical. The essential equations are presented and explained but not always fully derived, an approach which seems appropriate to this level of presentation. The chapters on energy calculations are followed by chapters on what modelers do once an energy surface has been obtained: minimization procedures, locating transition states, and molecular dynamics (MD) and Monte Carlo (MC) simulation. In each case there is a strongly utilitarian thread, essentially what needs to be explained to a new research student without going overboard. The author follows through admirably in providing informed perspectives on the choice of various methods applicable to a given problem: the various algorithms for first- and second-order energy minimization, alternative truncation schemes for long range interactions in simulation, and diverse techniques for conformational searches. In the chapter on conformational analysis, there are brief but nicely written overviews of more specialized techniques such as distance geometry, genetic algorithms, pattern recognition, and docking. Leading references are provided to sources, and a listing of computational chemistry web sites is included. The book concludes with chapters devoted to the special topics of free energy determination, solvation methods including Poisson−Boltzmann and generalized Born methods, and rational drug design.

Modeling, from conceptual to mathematical to computational, is an increasingly essential tool in the repertoire of the modern scientist. Molecular and macromolecular systems are just too complex to fathom at the level of detail at which "nature solves the Schroedinger equation", and explanation in molecular science is often linked with successful modeling initiatives. Molecular modeling via computational chemistry is a subject that has developed over the last 35 years, and has truly come of age in the 1990s thanks to team efforts to develop large suites of programs such as the Gaussian suite of programs for molecular quantum mechanics, MM2 for small molecules, AMBER, and CHARMM, and GROMOS for molecular dynamics and the remarkable impact of EXPLOR on crystallographic and NMR structure refinement. At this point, computational methods for developing accurate molecular models are being rapidly advanced with improvements in basis sets, correlation methods, force fields, and advances in computer technology. Current and future chemistry and increasingly biochemistry and molecular biology students will emerge from their undergraduate programs with modeling in their repertoire every bit as much as physical methods. Andrew Leach's useful and timely text is just the companion for those undertaking research with a computational chemistry component and seeking a basic introduction to methods, thoughtful definitions of terminology, and a proper context and informative perspective on the field in general. *Molecular Modeling*, in conjunction with a Hyperchem-based laboratory component, should serve well as a text in a special topics course in computational chemistry for advanced undergraduate students.

David L. Beveridge, *Wesleyan University*

JA965801+

S0002-7863(96)05801-5

Methods in Enzymology, Vol. 286: Lipases Part B Enzyme Characterization and Utilization. Edited by Byron Rubin (Lipomed) and Edward A. Dennis (University of California−San Diego). Academic Press: San Diego. 1997. $99.00. xxxi + 563 pp. ISBN 0-12-182187-0.

Chemists view lipases either as a pharmaceutical target or as a synthetic tool. Digestive lipases are a pharmaceutical target because a selective inhibitor may lead to an antiobesity drug. As synthetic tools, chemists exploit the high enantio- and regioselectivity of commercial lipases to make enantiomerically pure or selectively modified molecules.

This volume contains twenty-four reviews approximately equally covering three topics: lipases in lipid metabolism, assay and kinetics of lipases, and the use of lipases in organic synthesis. The first two topics are relevant mainly to the role of lipases as a pharmaceutical target. These sections include articles on the role of lipases in lipid absorption and metabolism, lipase inhibitors, and monolayer techniques for kinetic measurements. The section on synthetic uses includes articles on screening techniques, molecular modeling, control of water activity and the effects of solvent on enantioselectivity. A companion volume, 284, *Lipases Part A Biotechnology*, covers the sequencing, cloning, and structural studies of lipases.

The authors are mainly European, reflecting expertise developed during the recent European Bridge Project on lipases (1990−93). The reviews give a good overview of the state of the art in lipase research. This volume is also an excellent starting point for researchers new to the field. There is some repetition, but this makes reading individual chapters easier. Several chapters lack a "procedure" which one expects from a methods volume. The references are up-to-date; most are from the 1990s.

Romas Kazlauskas, *McGill University*

JA975675P

S0002-7863(97)05675-8

Statistical Mechanics for Chemists. By Jerry Goodisman (Syracuse University). Wiley-VCH: New York. 1997. xi + 344 pp. $64.95. ISBN 0-471-16812-2.

The beauty of statistical mechanics is that it can be applied successfully to a whole range of problems commonly encountered in chemistry, physics, chemical engineering, and biophysics. Consequently, a wide range of texts exist which target these different audiences. Whatever the audience, one cannot escape the fact that students wishing to study the subject require a solid mathematical foundation, together with an understanding of probability theory, thermodynamics, and quantum mechanics. Hence, statistical mechanics is usually taught at the graduate level in most chemistry programs. Even at the graduate level it is difficult to obtain a good balance between mathematical rigor and interesting practical chemistry applications which will (hopefully) enlighten the student as to the full power and scope of the subject. This is one of the major aims of *Statistical Mechanics for Chemists*.

The author has developed a text suitable for a one or two semester graduate level course covering the principles of statistical mechanics, together with common applications in the field of chemistry. The book is well written and succeeds in presenting a difficult subject in a clear and straight forward manner. While not as comprehensive as *Statistical Mechanics* by McQuarrie, it has the advantage of including more of the mathematical steps explicitly in the text, thereby removing many of the mathematical manipulations which often intimidate chemistry graduate students.

The book consists of eight chapters, each of which is followed by a set of thirty or so problems. The overall content of the book is typical

of other texts in the area. The first two chapters provide the usual background concerning the mathematics of distributions and a review of thermodynamics, followed by the introduction of the concept of ensembles and fluctuations and their relationship to thermodynamic parameters. Chapter three is focused on the treatment of independent particles (ideal gas, crystal vibrations, spins in a magnetic field), while chapter four develops the partition function for molecules and includes applications for the treatment of chemical equilibria and adsorption (Langmuir isotherm). Quantum statistical mechanics is the subject of chapter five, concentrating on electrons in metals, semiconductors, and black-body radiation. Chapter six introduces classical statistical mechanics and how it can be used for the study of transport properties (heat conduction, diffusion, and viscosity), dipoles in a field, and dielectric properties of solutions. The liquid phase is introduced in chapter seven through the use of the virial expansion, cluster diagrams, distribution functions, and integral equations, leading into Debye−Hückel theory. The book concludes with a chapter on time dependence covering the Liouville equation, relaxation to equilibrium, time correlation functions, diffusion, the Langevin equation, and chemical reactions.

There are very few mistakes in the text, and the questions at the end of each chapter provide further practical applications of the different sections. Whether one should adopt this text for a graduate course in statistical mechanics will depend on your individual taste/bias. For instance, some of the subjects not covered in this book (and not necessarily in any of the other common texts either) include statistical mechanical perturbation theory, thermodynamic integration, molecular dynamics and Monte Carlo simulation techniques (mentioned only briefly considering they have been the major tools used for the development of statistical mechanics in the last three decades), Kirkwood−Buff theory, phase transitions (Ising models), and the statistical mechanics of polymer chains. In addition, some of the sections could have been improved slightly by including a critique to aid the student (Debye−Hueckel theory, different integral equation closures, in particular). However, these are minor points concerning what is a particularly interesting book for the general chemistry graduate student.

Paul E. Smith, *Kansas State University*

JA9756477

S0002-7863(97)05647-3

Hypervalent Iodine in Organic Synthesis. By Anastasios Varvoglis (Aristotelian University of Thessaloniki, Greece). Edited by A. R. Katritzky (University of Florida−Gainesville), O. Meth-Cohn (University of Sunderland), and C. W. Rees (Imperial College of Science and Technology−London). Academic Press: San Diego. 1997. xix + 223 pp. ISBN 0-12-714975-9.

Organohypervalent reagents have become an important class of chemical compounds which in many cases are the reagents of choice for various synthetic transformations. Professor Varvoglis has contributed substantially to this area of research and has also written a number of reviews as well as an earlier book on the subject. His earlier book, *The Organic Chemistry of Polycoordinated Iodine* (1992), covered the entire field while the present work focuses on applications in organic syntheses. While there is some overlap, new material is presented and some excellent examples are given of critical uses of these reagents. The twelve chapters which constitute the contents present preparative methods followed by chapters devoted to synthetic applications of the reagents. An introductory chapter titled general considerations lists most of the important reviews on hypervalent iodine chemistry. The first reagent covered is (diacetoxyiodo)benzene, and a detailed experimental section is given for its use in the conversion of 1,5-cyclooctadiene to 2,6-diacetoxybicyclo[3,3,0]octane. A number of other applications are given with actual experimental details. These include the oxidation of ketones to yield α-hydroxydimethyl acetals, the 1,4-oxidative fragmentation of α-stannylated lactols, the oxidative cyclization of lactols, and the oxidation of various nitrogen compounds. The literature coverage is quite complete and accurate. The succeeding chapters, [Bis(acyloxy)iodo]benzenes, Iodosylbenzene, (Difluoroiodo)- and (dichloroiodo)arenes, [Hydroxy(tosyloxy)iodo]benzene and Its Analogues, Diaryl Iodonium Salts, Phenyliodonium Salts with an Aliphatic Moiety, Phenyliodonium Zwitterions, Reagents of Iodine(V), and Some Further Reagents of Iodine(III), are in the same format and are equally useful. Particularly noteworthy is the presentation of the Dess−Martin reagent which includes the important observation of Meyer and Schreiber in 1994 that a small amount of water is in fact useful although the original description recommended anhydrous conditions. This degree of synthetic awareness makes the book particularly useful. References to the use of this reagent as late as 1995 are given.

I can strongly recommend this book. It should have a wide audience among organic chemistry. It is written at a level appropriate both for graduate students and people working in synthetic organic chemistry. This book accomplishes the dual goal of presenting organohypervalent iodine reagents in a descriptive way, and by virtue of the inclusion of actual experimental procedure, it becomes a valuable reference text.

Robert M. Moriarty, *University of Illinois at Chicago*

JA975507X

S0002-7863(97)05507-8

Advances in Molecular Structure Research, Vol. 2. Edited by Magdolna Hargittai (Hungarian Academy of Sciences) and Istvan Hargittai (Budapest Technical University). JAI Press: Greenwich. 1996. ix + 255 pp. $109.50. ISBN 0-7623-0025-6.

This book is the second volume of a user-oriented series which discusses the progress in molecular structure research. What is particularly interesting about the book is the fact that it reviews the frontiers of this field, taking a critical approach to the feasibility of various calculations and to the reliability of results.

The first chapter discusses conformational principles of congested organic molecules, with emphasis on trans versus gauche stability.

The second chapter describes transition metal clusters from the point of view of molecular versus crystal structure.

The third chapter discusses a novel approach to hydrogen bonding, trying to answer the question, "which molecules are most likely to form the strongest hydrogen-bonds?", by developing a method which makes use of simple induction from experimental evidence.

Partially bonded molecules and their transition to the crystalline state are discussed in the fourth chapter.

The fifth chapter describes valence bond concepts, molecular mechanics, and molecular shapes with emphasis on the hybrid orbital strength function.

Empirical correlations in structural chemistry form the subject of the sixth chapter.

The seventh chapter deals with the NMR "inadequate" technique, while the eighth and last chapter proposes a complete mathematical solution for the study of conjugated polyene hydrocarbons.

The book is written in a concise yet comprehensive manner, and touches on a variety of subjects not discussed extensively elsewhere. It presents an exhaustive and critical coverage of the literature even though some of the references are somewhat dated.

This book is recommended for researchers interested in new points of view in structural chemistry.

Anne-Marie Sapse, *John Jay College*

JA9755828

S0002-7863(97)05582-0