several chapters is that figures are reproduced too small or without sufficient clarity to be useful. It mainly occurs when figures are taken from one of the references. In one or two cases, a figure with multiple lines is reproduced without a legend. Overall, this book provides a wealth of information in a rather narrowly directed area. It is not designed to be on the bookshelf of every chemist. The editor is correct in stating that it will be most useful to product development and applications engineers. For the most part, the book achieves its stated purpose, though somewhat unevenly.

Richard L. Kiefer, *College of William and Mary*

JA975649R

S0002-7863(97)05649-7

Chemical Reactions and Their Control on the Femtosecond Time Scale. Series: Advances in Chemical Physics, No. 101. Edited by Pierre Gaspard (University Libre de Bruxelles) and Irene Burghardt (University of Bonn). Wiley/VCH: New York. 1997. xxix + 947 pp. $145.00. ISBN 0-471-18048-3.

Chemical Reactions and Their Control on the Femtosecond Time Scale is based on the 20th Solvay Conference on Chemistry, a descendant of the early Physical Conferences of the Solvay Institute where the initial paradoxes of quantum mechanics were examined. This latest meeting also considered quantum problems, with a focus now on understanding, observing, and controlling chemical reactivity using molecular quantum dynamics. The resulting book is a sound compilation of modern photochemistry. Contained in this work are eight major sections describing laser control of chemical reactions, femtosecond probing of chemical reactions, intramolecular dynamics, ZEKE and transition state spectroscopy, molecular Rydberg states, photodissociation, and reaction rate theory. In all there are 28 chapters comprising the scientific portion of the book and several interesting historical overview chapters.

The work contains nearly 900 pages of current theoretical and experimental photochemical investigations of both gas and condensed phase systems. In each of the eight major sections there is at least one comprehensive chapter reviewing both the background and the state-of-the-art of the area under consideration. Each section also concludes with a general discussion between the participants where one obtains not only enlightening (and at times lively) points of view, but also copious figures, detailed explanations, and thorough referencing (concerning which there are easily more than 1200 throughout the work). The discussion sections are not pasteurized; hence, one obtains a genuine feel for the thread of the meeting. For instance, when the pessimism regarding the possible applications of laser control of large scale chemical reactions is noted on p 277, M. Quack recalls that the widely used technique of NMR grew directly out of the Stern−Gerlach experiment, an atomic beam experiment!

The book begins with two sections focused on femtochemistry that are essentially a summary of the experimental efforts of several groups to employ the concept of coherence both in the probing of chemical reactions in real time and in the production of some degree of control over actual chemical reactions. As presented in the report by Gerber, the original concept of selectively breaking a chemical bond in a polyatomic molecule by precisely exciting that bond with a CW (nanosecond) laser failed because of rapid energy redistribution throughout the remainder of the molecule. With a single laser frequency, one essentially heats the entire molecule. Using coherence, e.g. simultaneously exciting multiple states within a system with a well-defined phase (a coherent superposition), one can begin to watch molecules react in real time (a focus of Zewail's chapter) and produce selective chemical reactivity. Much of the first third of the book is concerned with experimental and theoretical descriptions of such coherent processes ranging from isolated molecules in the gas phase to small metal clusters, to larger clusters, to condensed phase systems. The femtochemistry sections end with a report by Fleming outlining perhaps the most interesting area on the ultrafast horizon, the fundamental considerations of chemical dynamics in the condensed phase.

Laser control of chemical reactions forms the next major section and begins with an outstanding overview of the field presented by Rice. The focus is on various perspectives of the control of quantum many-body dynamics, with specific application to chemical reactions. Included are lucid discussions of the Brumer−Shapiro method and the Tannor−Rice−Kosloff−Rabitz method of coherent control. Rice points out that the essentials of the two methods are identical in that quantum interference effects are at the core, but that each method emphasizes different aspects, the former focusing on the phase of two interfering pathways between an initial and final state and the latter focusing on manipulating the time difference between two frequency-shaped excitation pulses. Within this section are chapters detailing new control schemes involving degenerate continuum states, feedback control of quantum dynamics, and control by ultrashort infrared pulses. A provocative question raised after the Rabitz report on optimal control theory concerned whether one could simply employ high-resolution spectroscopic data to tailor the control pulse rather than relying on an empirical, iterative approach. The question remained unanswered after appearing time and again in the discussion sections. The discussions of laser heating, cooling, and transparency (Tannor) will be of interest to the uninitiated, and a comprehensive chapter on time-frequency and coordinate-momentum Wigner wave packets in nonlinear spectroscopy (Mukamel) will be of interest to the expert.

The remaining sections of the book are concerned more with chemical reaction theory than with specific control schemes or even femtosecond pump−probe experiments. None-the-less, inclusion of the sections on intramolecular dynamics, transition state spectroscopy, and reaction rate theory are crucial for the understanding and advancement of femtochemistry. The theory of chemical reactivity at low and high internal energies is presented by Marcus and Gaspard, respectively. Gaspard also sets the stage for the series of chapters on molecular Rydberg spectroscopy that follow. For the experimentalist, the chapters on ZEKE, photodissociation spectroscopy, coherent ion dip spectroscopy and ion−molecule reactions will be of interest. Intertwined with these are theoretical chapters explaining the novel aspects of experimental observations and other phenomena such as inverse Born−Oppenheimer states, resonances in unimolecular dissociation (transition state spectroscopy), and phase and amplitude imaging of evolving wave packets by spectroscopic measurements. Field's report details the correspondence between time and frequency domain investigations of intramolecular dynamics and presents the polyad method for "unzipping" spectra in highly excited molecules where intramolecular energy redistribution dominates. The book concludes with a section on reaction rate theories including chapters on statistical adiabatic channel calculations on state-specific dissociation dynamics and on quantum and semiclassical theories of chemical reaction rates by Troe and Miller, respectively.

While there is no doubt that many important aspects of modern photochemistry are addressed well in this work, perhaps more attention should have been paid to chemical reactions in the condensed phase. With that caveat, the interplay of premier theoreticians and experimentalists both during the 20th Solvay conference on Chemistry and in the preparation of the chapters results in a coherence that stamps this work as first class. The book should be of considerable value to photochemical aficionados and beginners alike.

Robert J. Levis, *Wayne State University*

JA975665O

S0002-7863(97)05665-5

Molecular Modeling: Principles and Applications. By Andrew R. Leach (Glaxo Wellcome R&D). Addison Wesley Longman: Essex. 1996. xvi + 595 pp. £35.00. ISBN 0-582-23933-8.

Molecular modeling calculations can now be performed in almost any chemistry classroom or laboratory. The current generation of commercial software such as Hyperchem for personal computers and Insight/Discover for workstation platforms has user-friendly graphical interfaces that make a diverse array of relatively sophisticated techniques readily accessible. A commonly voiced criticism is that making molecular modeling easy to use also makes it easy for a student or novice user to choose a wholly inappropriate technique or method for a particular problem. This problem can be readily overcome with better education for potential users. Andrew Leach's new book, *Molecular Modeling*: *Principles and Applications*, speaks directly and effectively to this issue.

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