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Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, *USA). As far as practicable, books will be reviewed in a country different from that of publication.*

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Reviews in computational chemistry. Vol. 3. Edited by K. B. LIPKOWITZ and D. B. BOYD. Pp. xvi + 271. Weinheim: VCH Verlagsgesellschaft, 1992. Price $75.00. ISBN 1-56081-619-8.

This book is the third in a series intended to provide a guide to the rapidly developing field of computer-aided research in chemistry. The book contains four chapters written by experts in the field. It covers optimization methods, the prediction of oligopeptide structures, molecular modelling using NMR data and methods for the evaluation of chemical toxicity. A fifth chapter provides a compendium of molecular modelling software. The book is intended to provide a tutorial to novices, and a review for experts, of the theoretical background, the implementation methods and the advantages and disadvantages of popular computational chemistry approaches.

A knowledge of optimization methods and their limitations is necessary for any structural chemist who plans to use computational methods. These topics are covered in chapter 1 (71 pp., 142 references) by Tamar Schlick of New York University. He covers essential aspects of the subject, beginning with mathematical preliminaries and moving to search techniques and local and global methods of large-scale optimization, with an explanation of local descent methods and several varieties of minimization methods. This exposition is followed by examples of the performance of various minimization routines. The chapter is comprehensive and, in principle, should provide the education needed by users. However, the explanations are couched in mathematical symbolism rather than in words so that, while the chapter will be useful to the expert seeking a review of methods and implementation strategies, the novice who wishes to understand the basic function of these methods may not be particularly well served.

Chapter 2 (69 pp., 251 references), by Harold Scheraga of Cornell University, is optimistically entitled 'Predicting three-dimensional structures of oligopeptides'. The chapter presents a detailed overview of the computational approaches adopted by the author and his co-workers, with only a cursory and generally critical discussion of alternative approaches to computing such structures or to solving the multiple-minima problem. There are summaries of the theoretical basis for the potential energy calculations used to predict structure, the build-up method of generating an oligopeptide chain and comparisons of computations with experimental observations. The presentation of the theory behind different potential functions and the methods available for treating hydration and entropy effects is clear, precise and useful.

Chapter 3 (49 pp., 121 references), by A. E. Torda and W. F. van Gunsteren of the ETH Zentrum, Zurich, presents the computational aspects of modelling a molecular structure based on nuclear magnetic resonance (NMR) data. The focus is on the determination of protein structure. The authors present the mathematical models for the experimental data and follow with an exposition of methods for refinement and minimization of the molecular model. They successfully bridge the gap between the novice reader and the expert, providing tuition for the former and a rich presentation of the state of the art of minimization and model development for the latter. The chapter provides a clear assessment of the errors and biases of the method and is instructive to the beginning user of molecular dynamics approaches. The presentation is clear and educational, and meets the objectives of the series.

Chapter 4 (49 pp., 227 references), by D. V. F. Lewis of the University of Surrey, presents computational approaches developed for the prediction of the toxicity of newly devel-

oped, untested chemicals. It is a good tutorial for the novice. A clear presentation of toxicology is provided and followed with excellent brief introductions to three computational approaches for toxicological study. Lewis clearly defines the parameters used in the traditional quantitative structure–activity relationship (QSAR) methods of Hansch, and explains pattern-recognition methods and knowledge-based systems. These methods are demonstrated and further explained by consideration of the P450 cytochromes and their role in toxic activation or detoxification of chemicals. Through this presentation, the author discusses several computer programs and their specific strengths. The chapter ends with a list of sources for these programs.

The editors conclude the book with a compendium of software, providing both a synopsis of and access information for 29 PC-based programs and 49 minicomputer or workstation-based programs for molecular modelling, quantum chemistry calculations, molecular graphics and molecular databases. This compendium is useful, but available in a much less expensive format from the Quantum Chemistry Program Exchange.

Overall, the book is elegantly presented and carefully edited. Two of the four chapters meet the stated aims of the series and provide a clear tutorial for novice readers. The book would be a useful addition to a research library; however, the lack of successful tutorial approaches for all four presentations makes it less desirable for a personal collection.

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Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Minerals and reactions at the atomic scale. Transmission electron microscopy. Edited by PETER BUSECK. (Reviews in Mineralogy, Vol. 27). Pp. xv + 508. Washington: Mineralogical Society of America, 1992. Price $28.00. ISBN 0-939950-32-4. The volume presents the proceedings of an MSA three-day short course, convened by the editor at College Corner, OH, in October 1992, on principles of electron microscopy and their application to aspects of mineralogy, petrology and geochemistry. There are 11 individual contributors to 12 chapters. Five of the 12 are devoted to principles and seven to applications. As well as for TEM, there are descriptions of SAED, CBED, EELS, ALCHEMI, high-resolution image simulation and X-ray analysis. Among the mineralogical applications described are the studies of polysomatism, polytypism, and chemical and structural definition and disorder in silicates. In petrology, applications to both low- and high-temperature and deformation-induced reactions are presented. Each chapter concludes with a comprehensive set of references to the original literature.

Electron crystallography. Edited by DOUGLAS DORSET. Pp. v + 182. Buffalo: American Crystallographic Association, 1994. Price $25.00. ISBN 0-937140-37-6. Volume 28 of the Transactions of the American Crystallographic Association, the book contains the proceedings of a symposium on electron crystallography held in conjunction with the annual meeting of the ACA at the University of Pittsburgh in August 1992. The book contains 15 presentations, by 36 different authors, and an editorial preface. Available from Polycrystal Book Service, PO Box 3439, Dayton, OH 45401, USA.

The structural chemistry of silicates. Edited by ADRIAN WRIGHT. Pp. xviii + 329. Buffalo: American Crystallographic Association, 1993. Price $25.00. ISBN 0-937140-36-8. Volume 27 of the Transactions of the American Crystallographic Association, the book contains the proceedings of a symposium on the structural chemistry of silicates, held in conjunction with the annual meeting of the ACA at the University of Toledo, OH, in July 1991. The volume contains transcripts for 13 of the invited and 11 of the contributed talks, including the Society of Glass Technology lecture delivered by John M. Parker, and five of the poster presentations offered at the symposium, The symposium was dedicated to the memory of the late Doris L. Evans and contains an appreciation of her work in silicate science, given by Michael P. Teter. Available from Polycrystal Book Service, PO Box 3439, Dayton, OH 45401, USA.

Linear and nonlinear optical properties of molecules. By G. H. WAGNIÈRE. Pp. xii + 196. Weinheim and Basel: VCH mbH and Verlag Helvetica Chimica Acta, 1993. Price DM 88.00. ISBN 3-527-29045-1. This is a concise enumeration and general treatment of the phenomena and principles of molecular optical spectroscopy, with particular emphasis on the molecular properties contributing to the various interactions of molecules with light, alone and in combination with static electrical and magnetic fields. The more detailed mathematical formalisms are placed in appendices that occupy rather more than half the text. A useful overview for the non-specialist and new students in the field.