# *Book Reviews*

**Reviews in Computational Chemistry. Volume 13**. Edited by Kenny B. Lipkowitz and Donald B. Boyd. Wiley-VCH, New York. 1999. xxxiii + 426 pp. 16 × 24 cm. ISBN 0471-33135-X. $135.00.

This volume of *Reviews in Computational Chemistry* is of the same very high standard as previous volumes. The editors have played a key role in carving out the discipline of computational chemistry, having organized a seminal symposium in 1983 and having been the chairmen of the first Gordon Conference in Computational Chemistry in 1986. Thus, they have a broad perspective on the field, and the articles in this and previous volumes reflect this.

This volume has a preface describing a recent Institute of Scientific Information Survey of citations in chemistry and the fact that, although computational chemists make up only 5% of chemists, they make up 25% of the 50 most highly cited chemists. They also discuss some aspects in the careers of two of the most prominent computational chemists, Lou Allinger and the late Michael Dewar.

There are six chapters in this volume. The first, by Bally and Bordon, is entitled Calculations on Open-Shell Molecules: A Beginner's Guide. This, like many previous chapters in this series, is a beautiful piece of pedagogy. This chapter should prove invaluable for many computational chemists who mainly work on closed-shell systems as well as for noncomputational types who want to learn about what calculations on radicals and biradicals can tell us about such molecules that would be of interest to the practicing chemist. The strengths and weaknesses of restricted and unrestricted Hartree−Fock approaches and the pitfalls sometimes encountered when one combines unrestricted methods with many body perturbation approaches are emphasized. This is an invaluable guide for the calculational state of the art in this area of quantum chemistry.

The second chapter, by Kestner and Combariza, is entitled Basis Set Superposition Errors: Theory and Practice. This chapter also deals with some thorny technical issues related to ab initio electronic structure calculations. Basis set superposition error (BSSE) occurs when one carries out calculations on two systems with the basis sets used to describe the wave functions not perfectly complete, which is true in every real system. How best to correct for this error is the question, and there have been many debates in the literature over the last 30 years on how best to carry out this correction. The use of localized orbitals seems to help in reducing the artefacts, but as noted by the authors, the simple counterpoise correction works reasonably well in many cases; however, when one uses non-atom-centered basis functions or is dealing with excited states, there are still unresolved issues. This chapter is timely and interesting and should be useful to those who carry out ab initio calculations on intermolecular interactions.

The third chapter, by Anderson, is Quantum Monte Carlo: Atoms, Molecules, Clusters, Liquids and Solids. This method describes the "third way" of solving the Schroedinger equation "ab initio", in additional to the more traditional approaches (Hartree−Fock + some method of adding correlation or density functional methods) emphasized in the first two chapters. For small systems, the quantum Monte Carlo (QMC) approach is the most accurate and has provided close to exact energies for the potential surface for the $H + H_2$ reaction. This chapter gives a sense of the state of the art of this method, i.e., what systems it can be applied to, and concludes with an analysis of the transition state for cyclooctatetraene bond shifting, where apparently versions of the two more traditional approaches cannot correctly order the singlet and triplet transition states, but QMC reproduces their energies to within 2 kcal/mol. This is an eye-opening chapter for someone who has mainly followed the two standard quantum chemistry approaches.

The fourth chapter, by Wallqvist and Mountain, Molecular Models of Water: Derivation and Description, describes both quantum mechanical and classical mechanical approaches to studying water interactions in gas, liquid, and solid. This chapter is very valuable for both its historical overview and its breadth in covering a wide variety of approaches. The emphasis is on pure water, so studies of solutions are not covered in great depth. Nonetheless, a person can get a good grounding in the way water potentials are developed and evaluated from this chapter. Unfortunately, some of the equations in this chapter are messed up but can roughly be figured out from context.

The fifth chapter, by Briggs and Antosiewicz, is entitled Simulation of pH-Dependent Properties of Proteins Using Mesoscopic Models. This chapter focuses on the calculations of the protonation states of ionizable groups in proteins, mainly concentrating on continuum approaches. This is a very valuable chapter, with well-written sections on the basic theory, how the theory is applied in practice, how experimental p$K_a$'s are determined, and finally sample applications and comparisons of different methods as to how well they reproduce the experimental p$K_a$'s in hen egg white lysozyme.

The final chapter, by Helson, describes Structure Diagram Generation, the process by which two-dimensional coordinates are generated from a connection table. This might seem a trivial task but is far from being so, and Helson's chapter describes well both the historical development and the importance of efficient computational methods to solve the problem of generating the two-dimensional representations from different starting points. Although outside my area of expertise, I found this chapter an enjoyable read.

All in all, this is a most valuable and well-written volume of chapters, covering a wide range of important topics in computational chemistry. More information on

*Reviews in Computational Chemistry* can be found at http://chem.iupui.edu/rec/rcc.html.

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supplement together with the complete series of *Rodd's Chemistry of Carbon Compounds* is highly recommended.

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**Second Supplements to the Second Edition of *Rodd's Chemitry of Carbon Compounds*. Volume IV: Heterocyclic Compounds. Part I. Six-membered Heterocyclic Compounds with Two Hetero-Atoms from Group V of the Periodic Table: the Pyridazine and Pyrimidine Groups. Part J. Six-membered Heterocyclic Compounds with Two Hetero-Atoms from Group V of the Periodic Table: the Pyrazine Group, Phenoxazine, Phenothiazine, Phenazine and Sulphur Dyes. Six-membered Heterocyclic Compounds with Three or More Hetero-Atoms**. Edited by M. Sainsbury. Elsevier, Amsterdam. 2000. xiv + 299 pp. 15 × 23 cm. ISBN-0-444-82980-6. $183.50.

This volume comprises Chapters 42−47 in a secend supplement to the second edition of *Rodd's Chemistry of Carbon Compounds*. These topics were last reviewed in 1995, reflecting the level of current interest in six-membered ring heterocycles containing two nitrogen atoms. With one exception, each of the chapters has been written by the same author(s) who reviewed the topics for the first supplement, thus insuring a high level of continuity between the supplements. Pyridazines, cinnolines, benzocinnolines, and phthalazines are updated in Chapter 42 by Drs. Parrick, Shaw, and Mehta. Recent progress in pyrimidine and quinazoline chemistry is reviewed in Chapter 43 by D. T. Hurst, while pyrazines, quinoxalines, phenazines, and dibenzopyrazines are updated in Chapter 44 by K. J. McCoullough. Dyes derived from phenazine, oxazine, and thiazine and some sulfur dyes are reviewed in Chapter 45 for the first time in this volume by R. Bolton, who is a frequent contributor to other volumes in the series. Prof. S. Johne reviews quinazoline alkaloids in Chapter 46, and the volume is completed with D. F. O'Shea's review of six-membered ring compounds containing three or more heteroatoms in Chapter 47. Included in this last chapter are triazines, tetrazines, pentazine, and hexazine; six-membered rings with nitrogen and sulfur, nitrogen and oxygen, and nitrogen, oxygen, and sulfur; and six-membered rings with two or more oxygen and/or sulfur atoms.

Each chapter is a concise, highly readable, and informative review. Key literature citations and important reviews are given. A comprehensive subject index for the entire volume is provided. Organic and medicinal chemists interested in the properties, synthesis, and reactions of heterocyclic compounds should derive considerable benefit from this volume. Library access to this

**Potassium Ion Channels: Molecular Structure, Function and Diseases**. Edited by Yoshihisa Kurachi, Lily Yeh Jan, and Michel Lazdunzki. Academic Press, San Diego, CA. 1999. xxiv + 492 pp. 15 × 22 cm. ISBN 0-12-153346-8. $99.95.

This book provides an excellent synopsis of the latest developments in the understanding at the molecular level of various $K^+$ channel classes that are increasingly being examined as therapeutic targets. It is a collection of 25 chapters written by many of the leading experts in the field. The majority of the chapters comprise critical and in-depth reviews of recent developments in $K^+$ channel research, including biophysical properties of voltage-gated, calcium-activated, and the more recently discovered two-pore $K^+$ channels; molecular makeup and mutations of the cardiac-delayed rectifier $K^+$ channels; and assembly, distribution, and physiological and pathological regulation of inward rectifier $K^+$ channels including G-protein-gated $K^+$ channels and ATP- sensitive $K^+$ channels. A concise update is also provided on the large extended gene family consisting of two, four, and six transmembrane-containing potassium channels that have appeared in the genome of the nematode *Caenorhabditis elegans*.

Three chapters collectively provide an elegant overview of the makeup and genetic analysis of two major types of cardiac $K^+$ currents, Ikr (rapid delayed rectifier) and Iks (slow delayed rectifier), namely, the *KvLQT1*/*minK* and *HERG* genes, respectively, that have been linked to two forms of hereditary long QT (LQT) syndrome. Seven chapters are devoted to the various strong inward rectifier $K^+$ channels, including aspects of assembly, rectification, permeation, and regulation. Four chapters are dedicated to G-protein-gated $K^+$ channels (GIRKs), discussing channel gating by G-proteins and phosphatidylinositol phosphates, muscarinic receptor activation of cardiac $K^+$ channels, and pathophysiology of the GIRK channel mutation in the *weaver* mouse. Five chapters on ATP-sensitive potassium channels review the functional analysis of cloned subunits, pharmacology of potassium channel openers (KCOs), and cardiac $K_{ATP}$ channels relevant to ventricular arrhythmia and cardioprotection.

No separate sections are devoted to the pharmacological aspects of $K^+$ channels. Appropriate discussions of channel modulators are included where they are deemed appropriate, for example, the interactions of class III antiarrhythmic agents such as *dofetilde* and MK-499 with cardiac-delayed rectifier $K^+$ currents, KCOs such as *pinacidil* at the ATP-sensitive $K^+$ channel, and

polyamines at the inward rectifier channels. Inclusion of a chapter highlighting the structure of $K^+$ channel subunits would have been a worthwhile and fitting complement.

Although many of the authors of this book were participants in the International Symposium on Potassium Ion Channels held at Yamagata (Japan), this book is not a mere collection of meeting proceedings, nor is it intended to be an introductory overview for the novice. With a variety of $K^+$ channel gene products cloned, characterized, and correlated with native $K^+$ currents over the past decade or so, this book comes at an opportune time to provide a critical appraisal of the exciting developments in the $K^+$ channel arena. This compendium is recommended for any serious student of ion channels from pharmacology, biophysics, molecular biology, and medicinal chemistry. Researchers wishing to understand the biophysical and molecular aspects of the ever-increasing members of the various $K^+$ channel types and their therapeutic potential will benefit immensely from this book.

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