Book Review

Cis–Trans Isomerization in Biochemistry Edited by Christophe Dugave (CEA/Saclay, Gif-sur-Yvette, France). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2006. xvi + 354 pp. $190. ISBN 3-527-31304-4.

Thomas P. Sakmar

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BOOK REVIEWS

Cis−Trans Isomerization in Biochemistry. Edited by Christophe Dugave (CEA/Saclay, Gif-sur-Yvette, France). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2006. xvi + 354 pp. $190. ISBN 3-527-31304-4.

Most students of biochemistry are introduced to cis−trans isomerization (CTI) by performing a simple yet elegant experiment in which a solution of maleic acid upon exposure to light in the presence of a catalytic amount of bromine is converted to fumaric acid, whose formation is signaled by formation of a white precipitate. If only CTI reactions were all so straightforward! In reality, a plethora of diverse but related CTI reactions occurs in living systems—some are photochemical, some are catalyzed enzymatically, and some are spontaneous. These reactions are often overlooked or misunderstood by many professional biochemists. This excellent multiauthor volume is an attempt to bring all these processes together under a common thematic framework, and it largely succeeds in this goal.

Despite the earlier efforts of Turro in his classic text, *Modern Molecular Photochemistry*, and those of other authors, CTI in the context of biochemistry has gotten a bad rap. Perhaps biochemists disregard the principle of microscopic reversibility and assume that photochemical CTI reactions are all unidirectional. The first third of this volume should help to usher photochemical CTI reactions into the mainstream of biochemistry. Photochemical CTI systems are covered in a progression of chapters that highlight theory, experimental approaches focused on retinal-based proteins, and computational methods. CTI reactions in biological membranes, for which a systematic lipidomic approach to understanding the functional evolution of cell membranes is argued, are also covered. One notable omission in the coverage is the fascinating story of the enzymatic regeneration of 11-cis-retinal in the retinal pigment epithelial cells and Müller cells in rods and cones of vertebrates.

The book becomes even more relevant and timely as the many aspects of CTI in protein structure and activity are presented. After an excellent background chapter on the chemistry of restricted rotation of ester, amides, and related moieties, there are three well-crafted and detailed chapters on CTI in peptides and proteins. Proline CTI reactions underlie protein-folding pathways and can dictate protein stability. After a flurry of activity in the 1980s that included the discovery of the cyclophilins as the binding targets of cyclosporine A and other peptidyl prolyl isomerase enzymes, the field has undergone a recent resurgence as newer methods, notably NMR spectroscopy and simulations using computational molecular dynamics, are advancing the understanding of how certain CTI reactions influence protein biogenesis and intramolecular switching reactions that control cellular signaling networks. The multiauthored chapter on the CTI of amides unites a wealth of information on proline, substituted prolines, and pseudoprolines. The logical next chapter on peptidyl prolyl isomerases is comprehensive, with over 200 references, essentially all of which are from the past six to eight years. The final two chapters cover tunable photoligands and CTI in metal complexes and nicely tie into the book's opening section.

Topics of special interest are not neglected in this volume, as Dugave has attracted as contributors an international group of authors with diverse backgrounds and interests. The consistency among the various chapters, often a challenge in an edited work with many authors, is enhanced by the fact that some authors have made final edits after reading drafts of the other's chapters. CTI reactions in biochemistry are more than just a curiosity, and this book merits addition to the library of any biochemist or chemical biologist interested in the role of fine structural detail in understanding dynamic biochemical reactions.

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The Quantum Theory of Atoms in Molecules: From Solid State to DNA and Drug Design. Edited by Chérif F. Matta (Mount Saint Vincent University, Halifax, Canada) and Russell J. Boyd (Dalhousie University, Halifax, Canada). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2007. xxxviii + 528 pp. $200. ISBN 978-3-527-30748-7.

This book covers the fundamentals and applications of Richard Bader's Quantum Theory of Atoms in Molecules (QTAIM). Over several decades beginning in the 1960s, Bader has pursued a course of thought directed at placing chemical concepts on firmer physical ground. Schrödinger had already developed his theory of the wave equation from a Lagrangian variational principle wherein his derivation assumed a surface term was zero, since the whole-system wavefunction goes to zero on the distant boundaries. That assumption led directly to the time-independent Schrödinger equation. Related variational approaches were further developed by Dirac, Feynman, and Schwinger.

Bader's QTAIM applies the Schwinger variational approach to an atom in a molecule, an inherently open system. Thus the surface terms discarded by Schrödinger must be retained, and zero-flux boundary conditions for that surface term are a basic aspect of Bader's theory. The QTAIM provides an unambiguous definition of what it means to be an "atom in a molecule". Using these ideas, Bader showed that the topological properties of the electron density (obtained from the gradient and Laplacian of the density) yield a great deal of information about structure, bonding, and reactivity in molecules. A notable aspect of QTAIM is that it is based on a *measurable* quantity, the electron density, and does not rely on chemical notions such as hybridization, etc. In 1990, Bader published the book *Atoms in Molecules: a Quantum Theory*, which lays out the fundamentals of this theory.

Unsigned book reviews are by the Book Review Editor.

The present book is a progress report 17 years later. It begins with an introductory summary of the theory and some preliminary applications. The book is then divided into five topical areas: (1) advances in theory, (2) solid state and surfaces, (3) experimental electron densities and biological molecules, (4) chemical bonding and reactivity, and (5) application to biological sciences and drug design. In the section on theory, Bader has contributed a concise chapter on the development of his approach in clear language. He also makes some predictions about future directions. This chapter can be recommended as a good starting point for someone new to QTAIM. Subsequent chapters in this section cover applications of QTAIM in the theory of atomic response properties, Raman scattering intensities, partitioning of molecular exchange energies, and the electron localization function.

The remainder of the book concerns a wide array of applications of QTAIM over the whole breadth of chemistry, materials, and biology. Applications discussed include bonding in molecular crystals, semiconductor surfaces, the topology of the electron density in solids, active sites on surfaces, the analysis of the electron density in complex systems such as proteins, transferability, fundamentals of chemical bonding and reactions in inorganic and organic chemistry, aromatic systems, hydrogen bonding, and drug design based on QTAIM descriptors. It is clear that what some might have considered an esoteric theory has culminated in a significant change in the way many think about chemical science. It is a refreshing lesson for young scientists to see such a recent theoretical development lead to new chemical thinking in an era that can sometimes be dominated by applications. The fact that it often takes decades for new ideas to bear fruit is also noteworthy!

The chapters are uniformly well written, and the authors maintain a consistent tutorial level throughout the book. This is an advantage for such an overview, where there is often a wide disparity in the way different authors approach their audience. I would highly recommend this volume as a good entry into the theory and applications of the QTAIM approach. Both the theoretical background literature and numerous applications are widely referenced, so the reader can pick and choose various topics of interest for further study.

Bader's original book was a clear exposition of the fundamental theory behind QTAIM. The present volume shows the influence of QTAIM throughout chemical science. I hope that this theory will make its way into freshman and physical chemistry textbooks in the future and replace some older ways of thinking with more physical approaches to chemical bonding and molecular interactions.

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Biochemistry and Molecular Biology Compendium. By Roger L. Lundblad (Consultant, Chapel Hill, NC). CRC Press/Taylor & Francis Group: Boca Raton, FL. 2007. x + 410 pp. $99.95. ISBN 1-4200-4347-1.

According to the Preface, the idea for this book arose when the author was revising *The Practical Handbook of Biochemistry and Molecular Biology* edited by the late Gerald Fasman. It occurred to him that much of the language and underlying concepts associated with biochemistry and molecular biology were not always well understood by students and practitioners in the field. This book, therefore, was designed to be a practical resource concerned with the "roots of biochemistry". It provides listings of commonly used acronyms and abbreviations along with their definitions; terms used in the field and related disciplines; commonly used chemicals and their properties; Log P values, water solubility, and molecular weight for selected chemicals; protease inhibitors and protease inhibitor cocktails; buffers; and organic name reactions useful in biochemistry and molecular biology. An extensive subject index completes the book.

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Reviews of Reactive Intermediate Chemistry. Edited by Matthew S. Platz (The Ohio State University, Columbus, OH), Robert A. Moss (Rutgers University, New Brunswick, NJ), and Maitland Jones, Jr. (Princeton University, Princeton, NJ). John Wiley & Sons, Inc.: Hoboken, NJ. 2007. x + 472 pp. $115. ISBN 978-0-471-73166-5.

This book is a second volume on the topic of reactive intermediates edited by Platz, Moss, and Jones and represents a timely addition to the first one, *Reactive Intermediate Chemistry*, that appeared in 2004. The present contribution is significantly smaller, with 10 chapters and nearly 500 pages, but it fills in some important gaps in the nearly encyclopedic coverage of reactive intermediates, methods for their study, and applications presented in the first volume.

In Part 1, there are two reviews of intermediate species not covered previously, in particular tetrahedral and pentacoordinate intermediates and intermediates derived from the elements silicon, germanium, and tin. These reviews are generously referenced up to 2005, and for practitioners in these fields, they should become valuable reference points for the synthetic and mechanistic understanding of these classes of reactive intermediates.

Part 2, which constitutes nearly three-fourths of the book, focuses on experimental methods and applications of reactive intermediate chemistry. This is effectively a reversal of the distribution in the first volume, where three-fourths of the text was devoted to a broad-ranging review of 16 important classes of reactive intermediates. The three chapters on methods provide an excellent introduction for both graduate students and more advanced readers to time-resolved resonance Raman spectroscopy, time-resolved infrared spectroscopy, and thermochemical measurements using mass spectrometric techniques. The chapters on applications are up-to-date reviews of the roles of reactive intermediates in combustion, crystals, and DNA damage. Finally, there are two theoretical chapters. The first addresses the role of conical intersections between excited electronic states as reactive intermediates, and the second is a discussion of quantum mechanical phenomena in organic intermediates.

I found all the reviews to be well written with up-to-date references, in some cases up to 2006. The editors have continued the prior format of also providing suggested readings of other appropriate texts and reviews along with detailed references, a

valuable feature for those wishing to further immerse themselves in the topics under discussion. This volume is an important complement to the previous one and should become a valuable resource for chemical researchers interested in a field that continues to represent one of the important frontiers of chemistry.

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Fourier Transform Infrared Spectrometry, 2nd ed. By Peter R. Griffiths (University of Idaho, Moscow) and James A. De Haseth (University of Georgia, Athens). J. Wiley & Sons, Inc.: Hoboken, NJ. 2007. xviii + 530 pp. $ 115. ISBN 978-0-471-19404-0.

One is always delighted by the opportunity to review an updated classic. This reviewer recommends with the highest enthusiasm the second edition of *Fourier Transform Infrared Spectrometry* to a wide spectrum of scientists. As was the case for its 1986 predecessor, this work is essential to all those interested in FT-IR. Graduate students, casual users, and practicing specialists will all find gems here to enhance their knowledge and appreciation of the technology, including, and perhaps most importantly, its limitations. The authors correctly note that the ease of operation of modern IR spectrometers is such that many users of these instruments have received little formal training in the field. This approach may be adequate as long as the measurements undertaken are routine but will cause difficulties when strange results are obtained, arising from either deterioration in instrumental performance or unusual samples. Thus, the authors' stated (and elegantly achieved) goal is not to provide a "compendium of all applications" but to describe the theory and instrumentation of FT-IR as it stands today. For those interested, applications have been reviewed comprehensively in the monumental "Handbook of Vibrational Spectroscopy" series co-edited by Chalmers and Griffiths.

The organization of this book is logical. The first 10 chapters provide a thorough, but not overly mathematical, introduction to the theory of vibrational spectroscopy and interferometry, followed by the basic features of sampling of the interferogram and the rudiments of Fourier transformation. Although it seems fair to note that some of the initial sections have been retained more or less intact from the prior edition, the authors have added substantively to the sections on modern approaches to interferometer design, photometric accuracy, and quantitative analysis. The initial introductory parts are supplemented with beautifully presented sections on the "nuts and bolts" of the practice of FT-IR, including components of the spectrometer and signal-to-noise ratio.

Whereas the introductory material retains the essence of the initial edition, most, if not all, of the sections on applications are either completely new or have been extensively revised with updated references. For example, the section on microspectroscopy and imaging provides a useful guide to what is probably the most exciting new direction of IR spectroscopic technology. Similar changes have been made to most of the remaining sections on applications, including those on time-resolved spectrometry, polarization, attenuated total reflection, photoacoustic, Fourier transform Raman spectrometry, and sample modulation spectrometry.

The beauty of this volume is that it integrates within a single source many elements not found elsewhere and, thus, fulfills the authors' aims. The level at which the material is presented is easy enough for beginning workers to understand, yet sufficient references to specific applications are included for the individual seeking greater detail on a particular topic to make his or her own way into the literature.

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