Reviews in Computational Chemistry, Volume 22 Edited by Kenny B. Lipkowitz (Howard University, Washington, DC), Thomas R. Cundari (University of North Texas, Denton), Valerie J. Gi...

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J|A|C|S
BOOK REVIEWS

Nomenclature of Inorganic Chemistry. IUPAC Recommendations 2005. Prepared for publication by Neil G. Connelly (University of Bristol, UK), Ture Damhas (Novozymes A/S, Denmark), Richard M. Hartshorn (University of Canterbury, New Zealand), and Alan T. Hutto (University of Cape Town, South Africa). International Union of Pure and Applied Chemistry and the Royal Society of Chemistry: Cambridge. 2005. xii + 366 pp. $150.00. ISBN 0-85404-438-8.

This book, also known as the "Red Book", is the definitive guide for internationally approved nomenclature for inorganic compounds. It updates the previous edition, which was published in 1990, and is also consistent with the principles of the IUPAC nomenclature for organic chemistry.

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Interphases and Mesophases in Polymer Crystallization II and III. Advances in Polymer Science, 181 and 191. Edited by Giuseppe Allegra (Politecnico di Milano, Italy). Springer: Berlin, Heidelberg, New York. 2005. xiv + 204 pp. $199.00. ISBN 3-540-25344-0 (for II). xiv + 304 pp. $259.00. ISBN 3-540-28280-7 (for III).

By offering various, and sometimes conflicting, viewpoints, these volumes, like the preceding one, attempt to shed some light on our understanding of how polymer crystals are formed. The focus of Volume 181 (and 180) is on "several basic aspects of morphology, inter-phase structure and disorder", whereas Volume 191 addresses such issues as "molecular interactions, modeling, phase transformation, and crystallization kinetics", to quote from the preface. Both volumes contain an index of all authors from Volume 101 to the volume in question, and both also include a comprehensive subject index for Volumes 180, 181, and 191.

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Organic Light-Emitting Devices. Edited by Klaus Müllen (Max-Planck-Institut für Polymerforschung) and Ullrich Scherf (Bergische Universität Wuppertal): Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2006. xviii + 410 pp. $170.00. ISBN 3-527-31218-8.

In 1987, Tang and Van Slyke demonstrated that organic materials are capable of electroluminescent behavior, and in 1990 Friend et al. fabricated the first polymer-based organic light-emitting diode (OLED). Ever since then, the area has experienced a "radiant growth", and an enormous number of publications dealing with OLEDs have appeared. It is thus timely to have this very impressive book, which the editors, both world experts in conjugated polymers, have assembled in order to illuminate all aspects of OLEDs.

There are 12 chapters, each written by leading experts in their field. The book starts with an instructive chapter about inorganic light emitting diodes (LEDs), which is an excellent way to compare currently employed technologies and their issues in a mature field to the emergent field of organic LEDs. The following, superb, chapters by Friend and co-workers and by Hertel and Bässler are investigations of the basics of organic heterojunctions and the spectroscopy of organic materials. In the next chapter, Heeger and co-workers discuss the applications of LEDs in array-type applications.

As an organic chemist, I was particularly interested in the chapter on the synthesis of electroluminescent polymers by Grimsdale. He gives a well-written overview of the field that should be an excellent entry to this area for both nonspecialists and advanced students. Aspects of charge-transporting and charge-blocking amorphous materials are discussed in the next chapter by Shirota, and specific techniques and specific classes of materials, e.g., dendrimers (Lupton), electrophosphorescent LEDs (Yang and Neher), are informatively presented in two of the remaining chapters that should also be useful to both nonspecialists and seasoned researchers.

Overall, this book gives an excellent overview of the field of organic light-emitting diodes. While it appeals to the specialist, the didactically smart structure makes it very useful and easy-to-read as well as enjoyable for the nonspecialist and graduate student. The chapters are well written, and the book is informative with up-to-date references and novel developments. I think the editors did an excellent job of putting this exciting volume together. All libraries and everybody interested in LEDs should own this book, which I am convinced will become a hit.

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Reviews in Computational Chemistry, Volume 22. Edited by Kenny B. Lipkowitz (Howard University, Washington, DC), Thomas R. Cundari (University of North Texas, Denton), Valerie J. Gillet (University of Sheffield, UK), and Editor Emeritus, Donald B. Boyd (Indiana University−Purdue University at Indianapolis). John Wiley & Sons, Inc.: Hoboken, NJ. 2006. xxviii + 362 pp. $160.00. ISBN 0-471-77938-5.

This volume consists of five chapters. The first four are concerned with topics related to protein folding, whereas the fifth is a discussion of wavelets applied to spectroscopic data processing and QSAR. In general, the aim of each chapter is to provide more of a tutorial introduction to the subject rather than a critical review of the field for experts. For those readers

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seeking more detail on a particular subject, there are many references citing the original literature over the past 30 years and more technical recent reviews.

The discussion in Chapter 1 addresses the comparison and classification of globular protein structures, including yet another derivation of how to calculate an optimal rigid-body superposition. There are many typos and grammatical errors marring the text, such as "triangular inequality" instead of "triangle inequality." The contents of Chapter 2 cover comparative/homology modeling as a regular how-to handbook full of examples, references, and URLs but not much critical analysis beyond warning about some common pitfalls. The authors' descriptions of some of the algorithms are utterly incomprehensible. The chapter reflects the state of confusion in the field, where there are enormous sequence databases and large numbers of experimentally determined three-dimensional structures, but there is little agreement about how to measure similarity with respect to sequence, structure, or biological function. Moreover, the causal or coincidental relation between sequence, structure, and function is even less clear, much less what connection there may be to real phylogenetic relations.

The thermodynamics and kinetics of protein folding are the topics of Chapter 3. While there are different theoretical analyses of these phenomena, the discussion here is strongly biased toward the school that draws an analogy between spin glass theory and protein folding. Although the authors are sometimes unclear about the distinction between potential energy and free energy, they do discuss many different levels of model detail, from one point per residue cubic lattice walks to all-atom off-lattice simulations with explicit solvent, and different algorithms for estimating folded structures as well as the kinetics of folding and unfolding. The very challenging numerical simulation of biological ion channels, including allusions to related problems in solid-state electronics, is discussed in Chapter 4. The authors reveal the "little-known" fact that "aqueous solutions ... are composed primarily of water molecules." Arguing that mainstream, explicit molecular dynamics of solvents is a hopeless way to simulate these channels, they concentrate on a detailed derivation of equations for a flux-based approach. Chapter 5 departs from the protein theme to cover wavelets vs Fourier transforms, the authors being apparently unaware of the use of wavelets to analyze protein structure. Their description of wavelets is not that clear, even for those who have dealt with them. The chemical applications offered concentrate on the analysis of spectra or developing quantitative structure−activity relationships. In the latter application, relatively few wavelet descriptors were required, but use of partial least squares was still necessary to sort out a reduced set of descriptors to a small number of different linear combinations of them.

Generally, the book gives a readable introduction to a wide range of topics regarding protein structure and folding and also to chemical applications of wavelets. For the reader who becomes more interested in one of these topics, there are many useful references to more technical reviews and the original literature.

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