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BOOK REVIEWS

Ionic Liquids in Organic Synthesis. ACS Symposium Series 950. Edited by Sanjay V. Malhotra (New Jersey Institute of Technology, Newark, NJ). American Chemical Society: Washington, DC (distributed by Oxford University Press). xiv + 306 pp. $184.50. ISBN 0-8412-7407-X.

This book was derived from a symposium of the same name held at the 228th National Meeting of the American Chemical Society at Philadelphia, PA in August 2004. There are 22 chapters, a sampling of which includes "Electrophilic Chemistry in Ionic Liquids", "Approaches to Imino Diels−Alder Reactions in Imidazolium Ionic Liquids", and "Tailoring Adsorption−desorption Properties of Hydroamination Catalysts with Ionic Liquids". An author index and a subject index complete the book.

JA0769651

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Chemoinformatics: Theory, Practice, and Products. By Barry A. Bunin (Collaborative Drug Discovery, San Mateo, CA), Jürgen Bajorath (Reinische Friedrich-Wilhelms-Universität, Bonn, Germany), Brian Siesel (Merrill Lynch & Co., San Francisco, CA), and Guillermo A. Morales (Telik Inc., Palo Alto, CA). Springer: Dordrecht. 2007. $129.00. xii + 296 pp. ISBN 978-1-4020-5000-8.

This book covers "the theory, commercially available packages and applications of Chemoinformatics", to quote from the Foreword. It was designed to be a practical handbook for computational scientists, medicinal chemists, and biologists to help them find the right technology for their purpose. The first section covers the theory of chemoinformatics, and the second is a discussion of its practice and products. Seventeen appendices follow, which are grouped under the headings: Drug Discovery Informatics Registration Systems and Underlying Toolkits; Content Databases; Drug, Molecule, and Protein Visualization; and Modeling and Algorithms. A subject index completes the book.

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Structure-Based Drug Discovery. Edited by Harren Jhoti (Astex Therapeutics, Cambridge, U.K.) and Andrew R. Leach (GlaxoSmithKline, Stevenage, U.K.). Springer: Dordrecht. 2007. xii + 250 pp. $169.00. ISBN 978-1-4020-4406-9.

Structure-based drug design (SBDD) is now an integral component of the drug discovery process. Nelfinavir (HIV-1 protease inhibitor), Trusopt (carbonic anhydrase inhibitor), Relenza (influenza neuraminidase inhibitor), and Celebrex (COX-2 inhibitor) are just a few SBDD success stories that have had a dramatic beneficial impact on human health. One of the latest developments in SBDD is the screening of fragment-based libraries.

Topics on the fragment-based approach to lead discovery form the core of the book and are described in Chapters 3−6. Chapter 3 by Leach and Hann would have served well as the lead-in chapter to the book because it presents a strong argument for the advantages of fragment-based screening relative to other methods of drug discovery. Unfortunately, the impact of this perspective is diminished by a subsequent chapter (6) by Zhang et al., who argue for an alternative scaffold-based approach. The distinction between fragment-based and scaffold-based seems to rely on a subtle difference in the definition of cutoff in molecular weights. As a result, these two chapters appear redundant. In fact, a common problem with the chapters on fragment-based screening is the repetitive descriptions of library design. Similarly, both the NMR and X-ray approaches to screening fragment-based libraries have been exhaustively reviewed in the literature.

The first two chapters present a progress report for the Joint Center for Structural Genomics (JCSG). Given the rapid development of structural genomics, the statistical details presented by Abola et al. will be quickly outdated. Furthermore, the high attrition numbers only illustrate a perceived disconnect between the immediate value of structural genomics and SBDD. Drug discovery programs do not operate by simply choosing a protein that readily crystallizes in a high-throughput assay. Instead, a better connection to SBDD should have been made by emphasizing how structural genomics is expanding the number of structures for therapeutic targets and how the technology developed for structural genomics is being adapted to SBDD.

An overview of the current challenges and limitations in molecular docking are described by Verdonk et al. in Chapter 8. This is a solid overview with an informative and well-described example that would have made a good introductory chapter to discussions on the roles of molecular modeling in fragment-based screening. Unfortunately this connection to fragment-based screening is missing, illustrating the lack of coherence in this book.

In Chapter 7, Chung and Lowe describe methodologies for measuring affinity constants, an important component of drug discovery. The authors were overly ambitious and tried to cover every major analytical technique. The result is a general, cursory list of methods that provides little insight, references, or illustrative examples. Similarly, the final chapter by Fenu et al. provides a comprehensive list of research focused on developing an optimal scoring function, a fundamental problem in molecular modeling and virtual screening. In an effort to be exhaustive, very little detail is provided that illustrates how the various approaches differ or how they are addressing a particular problem in a scoring function. Additionally, there are no

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examples that demonstrate the relative success or failures of any of the techniques.

The book's core subject matter of fragment-based screening is an exciting and important development in drug discovery. These chapters are generally the strongest in the book and make it a good reference volume, in lieu of collecting corresponding review articles from the literature.

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JA076951V

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Catalysis from A to Z: A Concise Encyclopedia, Volumes 1−3, Completely Revised and Enlarged 3rd ed. Edited by Boy Cornils (Hofheim, Germany), Wolfgang A. Herrmann (Technische Universität München, Germany), Martin Muhler (Ruhr-Universität, Bochum, Germany), and Chi-Huey Wong (Scripps Research Institute, La Jolla, CA). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2007. 1560 pp. $560.00. ISBN 978-3-527-31438-6.

The third edition of this popular and useful encyclopedia has been expanded to include approximately 8000 entries, compiled by more than 260 experts from around the world, as well as 3100 figures and 110 tables. It also contains 3300 cross-references and approximately 20,000 references in all. Special emphasis is on "the structures of catalysts and chemical compounds, reaction equations, and—wherever accessible—schemes of commercial and industrially proven processes ...", to quote from the Preface. Keywords are also given in German and in French.

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Columns for Gas Chromatography: Performance and Selection. By Eugene F. Barry (University of Massachusetts Lowell) and Robert L. Grob (Villanova University). John Wiley & Sons, Inc.: Hoboken, NJ. 2007. xiv + 298 pp. ISBN 978-0-471-74043-8.

This book is a practical resource for scientists and technicians working with packed column and capillary column gas chromatography. Authors Barry and Grob discuss the development, performance, selection, and technology of columns for gas chromatography and include a handy list of packed column separations and guidelines for column selection in Appendices A and B. A subject index completes the book.

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Activation of Small Molecules: Organometallic and Bioinorganic Perspectives. Edited by William B. Tolman (University of Minnesota, Minneapolis). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2006. xviii + 364 pp. $185.00. ISBN 3-527-31312-5.

As noted by Borovik and co-workers in Chapter 6 of *Activation of Small Molecules*, "[o]xidation chemistry has attracted the attention, and in many cases the passion, of chemists for well over a century." This statement is equally valid for small-molecule activation and its importance to the fields of synthetic inorganic, organometallic, and bioinorganic chemistry. This book provides a sweeping overview of the chemistry of metal-mediated small-molecule activation, with chapters organized by substrate (CO_2, NO and N_2O, N_2, H_2, O_2, CH_4, H_2O, and CO) and written by leading researchers in the field. As with any review by a collection of authors, this work shows stylistic differences from chapter to chapter, both in terms of organization and in the uniformity of figures, with little attempt to have ideas and concepts flow from one chapter to another. Despite these limitations, most chapters are well written with clear figures, contain primary literatures references through early 2006, and stand on their own admirably as a starting point for the subject material.

Oxygen is the one small-molecule substrate to receive more coverage than just one chapter in this book, and this expanded focus provides a nice comparison between two different strategies for reactions involving oxygen-based chemical oxidation. In Chapter 5, Cornell and Sigman provide an overview of organometallic O_2 activation. The authors cover various ligands, metals, and cocatalysts, paying particular attention to issues of selectivity in the oxidation of both simple and complex organic substrates. To complement this organometallic approach, Borovik, Zinn, and Zart present a bioinorganic perspective of O_2 activation in Chapter 6. Here, the authors focus on the oxidation state of the metal, electronic structure, coordination geometry and secondary structure in synthetic and biological O_2 activation, explaining how these factors lead to reversible binding or irreversible reaction of O_2 at the metal center. These chapters work extremely well together, giving the reader a balanced view of two approaches to the utilization of dioxygen in homogeneous oxidation reactions.

If the greatest strength of *Activation of Small Molecules* lies in the breadth of the material covered, this trait is also the book's greatest weakness. With the exception of the aforementioned chapters on O_2 activation, the general structure of the book allocates one chapter for each small-molecule substrate. While this approach allows for many small-molecule activations to be covered in one concise volume, it precludes a balanced treatment of any substrate, except O_2. For example, in Chapter 3, which is an excellent overview of N_2 activation and functionalization by Peters and Mehn, the authors focus on bio-inspired synthetic complexes of the group VI and VIII metals. The literature coverage is first-rate and includes the most current work from leading researchers in the field. Although Peters and Mehn provide insightful analyses of the structure−reactivity relationships in this area, a complementary chapter covering an organometallic approach would have provided the reader a more balanced view of the entire N_2 activation field. A similar comment generally applies to the other substrates covered in this monograph: *either* the organometallic or the bioinorganic approach is emphasized, with little or no discussion concerning the alternative approach. This is not a criticism of any individual chapter but rather a limitation imposed by the broad coverage of subjects in the book.

Activation of Small Molecules is an excellent text that introduces wide-ranging areas of small molecule activation as approached by experts in the fields of organometallic and bioinorganic chemistry. In such a concise volume, it would be impossible to assemble a comprehensive treatment of the area. In fact, entire volumes have been dedicated to each of the many substrates covered here. Nonetheless, given its broad coverage, this volume will be greatly appreciated by students and researchers looking to tackle new problems in small-molecule activation. In addition, for those working in the organometallic and bioinorganic fields, this text will be valuable as a desktop source of background and reference materials. It is highly recommended.

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Nanotechnology in Catalysis, Volume 3. Edited by Bing Zhou (Headwaters Nano Kinetix Inc., Lawrenceville, NJ), Scott Han (Rohm & Haas Company, Spring House, PA), Robert Raja (University of Southhampton, U.K.), and Gabor Somorjai (University of California at Berkeley). From the Series, Nanostructure Science and Technology. Series Edited by David J. Lockwood. Springer Science + Business Media, LLC: New York. xxii + 334 pp. $129.00. ISBN 0-387-34687-2.

This book is based on the symposium "Nanotechnology in Catalysis III" held at the 228th National Meeting of the ACS in Philadelphia, PA in the Fall 2004, although it does contain some chapters from authors who did not attend. Its 15 chapters are grouped into the following sections: New Concepts and Applications of Nanotechnology for Catalysis; New Methods, Structure and Understanding of Nanocatalyts; Nanoparticle Catalysts; and Nanoparticle Catalysts for Fuel Cell Applications. A subject index completes the book.

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Characterization II. From the series Molecular Sieves: Science and Technology, Volume 5. Edited by Hellmut G. Karge (Fritz Haber Institute of the Max Planck Society, Berlin, Germany) and Jens Weitkamp (University of Stuttgart, Germany). Springer: Berlin, Heidelberg, New York. 2007. x + 516 pp. $399.00. ISBN 978-3-540-30457-9.

This volume covers "a variety of non-spectroscopic techniques for the characterization of zeolites and related materials" and complements the previous one in the series, *Characterization I*, in which the emphasis was on spectroscopic techniques. The first four chapters cover methods of characterization, such as analysis by chemical, thermal, and ^{129}Xe NMR spectroscopic means, and the definition of pore size by molecular probes. The characterization of coke on zeolites and isomorphous substitution in zeolites form the topics of the remaining two chapters. An author index to Volumes 1−5 and a subject index complete the book.

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