J|A|C|S
BOOK REVIEWS

Artificial Enzymes. Edited by Ronald Breslow (Columbia University). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2005. xii + 182 pp. $99.95. ISBN 3-527-31165-3.

Despite the popularity of research in catalysis by artificial enzymes over the past several decades, this is the first book dedicated to an overview of the topic, although more comprehensive titles are available for specific classes of artificial enzymes. The book comprises seven chapters written by leading authors in the respective areas. The prose is uniformly literary yet accessible to those with limited knowledge in the field. The text is competently referenced with citations through early 2004, although the index is somewhat limited. No author index is provided, but one would have been a welcomed inclusion.

The chapters provide meaningful, albeit somewhat narrow, coverage of subjects ranging from purely synthetic catalysts to catalytic antibodies and protein-based catalysts to artificial restriction enzymes. The average chapter consists of roughly 25 pages, in which many of the authors have elected to highlight their own important contributions along with seminal efforts by other groups. This makes the information in each chapter readily digestible but offers somewhat superficial coverage of other important contributions outside the authors' own research. Also, little mention is made of either imprinted polymers or catalytic dendrimers, which are notable in both their design and implementation as enzyme mimics. Chapters dedicated specifically to these topics would have improved the scope.

Artificial Enzymes does serve as a highly readable introduction to this creative chemical discipline. It is certainly a worthy addition to the library of those new to biomimetic chemistry or to those who have lost touch with the field. It is also relatively affordable and fills a critical gap in the literature of bioorganic/supramolecular chemistry. However, its coverage may prove limited to researchers already intimately familiar with the subjects addressed.

Timothy Snowden, *The University of Alabama*

JA0598412

10.1021/ja0598412

Analytical Techniques in DNA Sequencing. Edited by Brian K. Nunnally (Wyeth Laboratories, Durham, NC). Taylor & Francis Group: Boca Raton, FL. 2005. xii + 238 pp. $189.95. ISBN 0-8247-5342-9.

There are 10 chapters in this multiauthor book that cover different analytical techniques of DNA sequencing, from the commonly used Sanger method to chip-based microfabricated sequencing systems. A large portion of the book is also devoted to various applications of sequencing, e.g., forensic DNA sequencing, genome analysis, sequencing the single molecule, etc. The book includes a short subject index and a thorough list of references at the end of each chapter.

JA0598661

10.1021/ja0598661

Computational Methods in Photochemistry. Molecular and Supramolecular Photochemistry, Volume 13. Edited by Andrei G. Kutateladze (University of Denver). CRC Press (an imprint of Taylor and Francis Group): Boca Raton, 2005. x + 518 pp. $179.96. ISBN 0-8247-5345-3.

I was eager to review this book as a way to learn about computational photochemistry, a field just outside my area of research. I was hoping for guidance on how to perform calculations of photochemical reactions, what techniques are most useful, and what pitfalls to avoid. Given this bias, the book was somewhat disappointing in that only two chapters of this multi-authored volume really address these issues: namely, the second chapter, "Computational Investigation of Photochemical Reaction Mechanisms", by Blancafort et al. and the fourth chapter, "Photochemistry from First Principles and Direct Dynamics", by Tonilo et al. In the first of these, the authors do a wonderful job of discussing the critical concept of conical intersections and excited-state potential energy surfaces—the authors have written other reviews on this same subject—whereas in the second, the authors discuss non-Born−Oppenheimer surfaces and direct dynamics. In both of these chapters, the authors attempt to walk the fine line between providing enough technical and mathematical detail to inform the reader of the subtleties of the problem without overwhelming the more casual reader. I am afraid that neither chapter quite achieves this difficult task; the less mathematically oriented chemist may find these chapters particularly turgid.

The remaining chapters present either case studies or special topics in photochemistry. The book is sandwiched by two chapters written by Zimmerman. The opening one is a survey of early applications of theoretical photochemical problems from the Zimmerman group. The closing chapter is a description of more recent work concerning theoretical studies of solid-state photochemistry. In between are chapters by Havlas, Kyvala, and Michl, who discuss spin−orbit coupling with a number of examples to related organic molecules, and by Gritsan, Platz, and Borden, who present a review of experimental and computational studies of nitrenes. While the latter chapter is up to the usual high standards of these authors, the bulk of this material has been presented in other reviews written by them. There is also a chapter on semiempirical MR-CI calculations in which Klessinger quickly covers the quantum mechanics to focus on how the method compares with more exact treatments. Finally, Weinhold describes the applicability of his natural bond orbital analysis to excited states, with the specific example of vinoxy radical.

Unsigned book reviews are by the Book Review Editor.

10.1021/ja0598412 CCC: $33.50

Although all of the chapters are well written, the book suffers from lack of coherency, the usual problem in books that have multiple voices. The book also contains more than its fair share of typographical errors, e.g., missing spaces, margins lost, and misspellings, making one wonder about the level of editorial care provided in creating the book. Overall, the book will likely be most useful when one of its specific chapters is of particular interest to the reader, but the book as a whole left this reviewer wishing for a fuller, more coherent treatment of the subject.

Steven M. Bachrach, *Trinity University*

JA0598715

10.1021/ja0598715

Macromolecules Containing Metal and Metal-Like Elements, Volume 7: Nanoscale Interactions of Metal-Containing Polymers. Edited by Alaa S. Abd-El-Aziz (The University of Winnipeg), Charles E. Carraher Jr. (Florida Atlantic University), Charles U. Pittman Jr. (Mississippi State University), and Martel Zeldin (University of Richmond). John Wiley & Sons, Inc.: Hoboken, NJ. 2006. xvi + 234 pp. $150. ISBN 0-471-68440-6.

Macromolecules containing metal and metal-like elements are broadly defined in this series as "large structures where the metal and metalloid atoms are (largely) covalently bonded into the macromolecular network within or pendant to the polymer backbone," whereas nanoscale means having "at least one phase dimension on the order of 1 to 100 nm". This volume contains four diverse reviews under this general umbrella, along with detailed outlines of each chapter and a lengthy index.

Belfiore and Fenton first describe how changes in macromolecular glass transition temperatures are controlled by coordination of metal complexes to ligands in the side group of the polymer. Fundamental concepts of coordination chemistry, such as ligand field theory, are described in detail; the intended audience appears to be polymer scientists rather than inorganic chemists. Schubert's chapter is a review of the synthesis of metal oxide clusters functionalized with polymerizable acrylate ligands and the properties of the resulting inorganic−organic composites. Carraher's brief description of metal-containing polydyes covers mostly older work and contains several typographical errors. The final review, by Pomogailo, comprises most of the volume. It covers the broad topic of "metallopolymer nanocomposite-macromolecular metallocomplexes as precursors for polymers, polymer inorganics, and bionanocomposites". Although this chapter contains a great deal of information on topics ranging from sol−gel composites to intercalated materials, as well as 813 references including several since 2000, the awkward writing style makes it difficult to read. There appears to be considerable overlap (including many of the same figures) with the author's recently published book *Metallopolymer Nanocomposites* (Springer, 2005), which covers similar topics in even more detail.

In summary, the book, perhaps in combination with other volumes in the series, may be useful to specialists in this interdisciplinary field with a background in either metal or polymer chemistry.

David S. Glueck, *Dartmouth College*

JA059879E

10.1021/ja059879e

Quantitation of Amino Acids and Amines by Chromatography: Methods and Protocols. Journal of the Chromatography Library, Volume 70. Edited by Ibolya Molnár-Perl (L. Eötvös University, Hungary). Elsevier B. V.: Amsterdam. 2005. xii + 654 pp. $274. ISBN 0-444-52050-3.

This book is a concise collection of the analysis of amines and amino acids by the various modes of separation. The authors lay out very well the progress that has been made in the analysis of these compounds by the various methods used over the years to the present. Whereas some of the references are dated in some of the sections, in others, there is excellent use of timely references to illustrate the current state-of-the-art. The authors do a very good job of pointing out both the traditional methods and the newer methods as well as examining the advantages and potential pitfalls of the various methods and protocols where appropriate.

The text is organized into sections that focus first on amino acids and then on amines. The sections are subdivided into the various separation methods, e.g., HPLC, GC, and electroseparations, and have a further focus separately on derivatized versus underivatized versions of these compounds. This style made the text very easy to follow and helped to make this book a handy reference.

In summary, I found the text overall to be a very useful collection of the various methods and protocols employed in the analysis of these very important compounds. The text is well organized and concise with timely references. It should serve as a handy and invaluable desk reference to novices and experts alike in the field of amine and amino acid analysis.

Jaycoda S. Major, *University of Rhode Island*

JA059837Q

10.1021/ja059837q

Theory and Applications of Computational Chemistry: The First Forty Years. Edited by Clifford E. Dykstra (Indiana University-Purdue University, Indianapolis, IN, USA), Gernot Frenking (Phillips-Universität Marburg, Germany), Kwang S. Kim (Pohang University of Science and Technology, Pohang, Republic of Korea), and Gustavo E. Scuseria (Rice University, Houston, TX, USA). Elsevier: Amsterdam. 2005. xxviii + 1308 pp. $110.00. ISBN 0-444-51904-1.

This book is a compendium of lectures presented at a conference on the theory and applications of computational chemistry held in Korea in February 2004. One presumes from the title and date of the conference that computational chemistry began around 1964. I recall using the first semiconductor chip-based computer at MIT around that time. Previously, we had to live with huge electric-tube diode systems. It was a relief to

see the considerable reduction in size and increase in speed of the new semiconductor machines, not to mention the decreased demand for cooling.

This book covers various themes of computational chemistry by various contributors—some well-known, some less well-known, and a few unknown. Overall, the quality is quite high, each author addressing the evolution of the subject close to his or her heart. Some reviews are exhaustive and thus pedagogical. Others are much too brief and could probably have been left out, a few examples being the newer areas, which were less well developed. For instance, Chapter 4 on electrodynamics could have provided a review of gauge problems, which have plagued early NMR theories and still remain a problem for current multiphoton processes; Chapter 8 on coherent control left out many of the current advanced numerical methods for undertaking computations in this new field; and Chapter 19 gave no indication why we would want to measure momentum densities, etc.

The book is saved by excellent reviews by Garrett and Truhlar on variational transition state theory (Chapter 5), Gerber et al. on multidimensional vibrational spectroscopy (Chapter 9), Hratchian and Schlegel on reaction paths (Chapter 10), Nakano et al. on density functional theory (Chapter 20), Scuseria and Staroverov on exchange-correlation functionals (Chapter 24), and Roos on multiconfigurational quantum chemistry (Chapter 25). The other chapters tend to overlap but are nevertheless complementary and thus allow the reader to bridge various methods and approximations.

Going through the chapter headings, one feels like the TV viewer who was told that different weather models were necessary at different times to follow Katrina, the already infamous hurricane that laid waste to New Orleans. Clementi's historical review (Chapter 6) was an interesting explanation for this meandering between various levels of approximation with time. As Clementi confesses, computational chemistry is a very vast field, and this book is testimony to the heroes who persevered so that today even industry has confidence in the latest methodology in computational chemistry.

There are some regrettable omissions: for example, time-dependent density functional theory; the theory of nuclear wave packet dynamics, which is evolving to electron dynamics due to the synthesis and characterization of attosecond (10^{-18} s) laser pulses; quantum Monte Carlo methods; and the advanced numerical methodology based on split-operators. Some of this work began about 10 years ago and could have been included to illustrate future trends. Notwithstanding this criticism, this is a useful book summarizing the failures and successes of computational chemistry. As the editors declare in the Introduction, this book should provide insights to where the field stands. Advances in hardware and algorithms have produced the remarkable power that computational chemistry holds and can do today.

André D. Bandrauk, *Université de Sherbrooke*

JA059883Q

10.1021/ja059883q