Additions and Corrections

Highly Electrophilic Olefin Polymerization Catalysts. Quantitative Reaction Coordinates for Fluoroarylborane/Alumoxane Methide Abstraction and Ion−Pair Reorganization in Group 4 Metallocene and "Constrained Geometry" Catalysts [*J. Am. Chem. Soc.* **1998**, *120*, 1772−1784]. PAUL A. DECK, COLIN L. BESWICK, AND TOBIN J. MARKS*

The electron affinity of the methyl radical used in Figure 4, quoted in a number of texts, has been superseded by a more reliable value.[1] A redrawing of Figure 4 with the more reliable value of E.A.($\bullet CH_3$) is shown below. The conclusion regarding metal and ligand contributions to ΔH_{dr} are unchanged; however, the new E.A.($\bullet CH_3$) value allows ΔH_{ips} to attain a magnitude more compatible with recent computational results.[2]

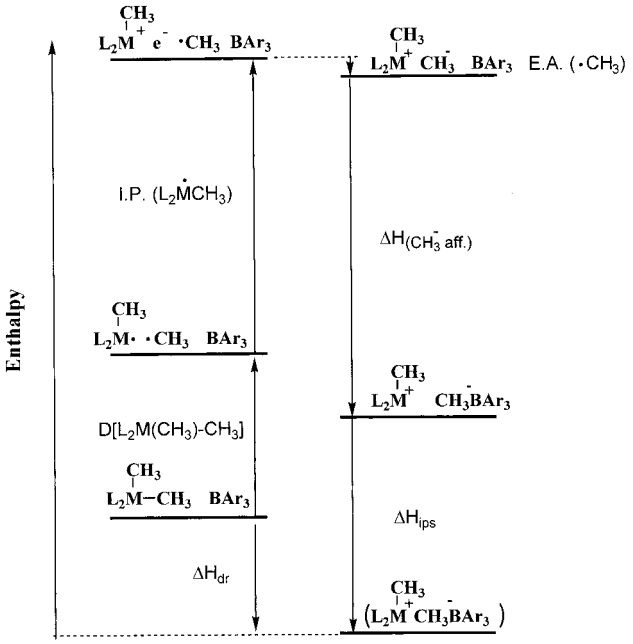

Figure 4.

(1) NIST Online Database, Chemistry WeBook, 1998, and references therein.
(2) Lanza, G.; Fragalá, I.; Marks, T. *J. Am. Chem. Soc.* **1998**, *120*, 8257−8258.

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Book Reviews

The Combinatorial Index. By Barry A. Bunin (AxyS Pharmaceuticals). Academic Press: San Diego. 1998. xvii + 322 pp. $79.95. ISBN 0-12-141340-3.

The synthesis and evaluation of small molecule libraries has undergone enormous growth over the past six years and is currently a central component of agrochemical and pharmaceutical research. Not surprisingly, an immense body of literature has appeared in numerous journals. Barry Bunin has written *The Combinatorial Index* to consolidate reliable small molecule library synthesis transformations from the primary literature into an organized and readily accessible format. He has succeeded admirably. *The Combinatorial Index* is the first book to provide a comprehensive, detailed overview of publications in the field. Summaries of experimental procedures enable critical evaluation of reported chemistry without requiring access to the primary literature.

The book is divided into six chapters. The first two chapters provide a brief background to the field. Chapter three then provides an extensive list of linkers for solid-phase synthesis in addition to an overview of general methods for functionalizing polystyrene supports. The detailed descriptions of linkers, which are categorized according to functional groups, are invaluable to combinatorial researchers since methods of substrate attachment to the support and the final cleavage of the products into solution are crucial features of all solid-phase synthesis strategies.

Chapter four provides procedures for carrying out important synthetic transformations on solid supports. Transformations are categorized as condensation reactions to prepare carbonyl derivatives and phosphorus compounds, carbon−carbon bond forming reactions, Mitsunobu reactions, substitution and addition reactions, oxidations, and reductions.

Finally, a large section of chapter four is devoted to the preparation of heterocyclic compounds due to the prevalence of heterocycle-based drugs.

Chapter five describes analytical methods that have greatly facilitated the development of solid-phase synthesis procedures. The first two sections are devoted to direct and indirect colorimetric methods for rapidly detecting the presence of functional groups, and in many cases, quantitating the exact amount of the functional group. The third and fourth sections are dedicated to the increasing number of NMR and IR techniques that have been developed to characterize support-bound compounds. The final sections provide examples of mass spectrometry and HPLC methods for the rapid characterization of compounds after release from solid supports.

Chapter six describes approaches to prepare libraries using solution-phase methods as well as a combination of solid-phase and solution-phase methods. The first section describes those methods that rely exclusively on library synthesis in solution. The second section describes a conceptually important approach for the purification of reaction products from reagents and reaction byproducts by "capturing" products on a support by reaction with support-bound functionality. The third and final section details the increasing number of support-bound reagents, catalysts and scavengers that have been utilized for the parallel synthesis of small molecule libraries.

The Combinatorial Index is a useful reference not only for the consolidation of published work, but also because of the excellent organization of the book. Four structural appendices divided according to functional group transformations, heterocyclization reactions, unnatural biopolymers, and oligosaccharides summarize the information provided in *The Combinatorial Index* and greatly facilitate access to the relevant material.

Bunin also maintains a World Wide Web site (http://www.combinatorial.com) that lists publications that have appeared after publication of *The Combinatorial Index* and are organized according to the table of contents of his book. Due to the vigorous activity in combinatorial chemistry, this supplement significantly enhances the utility of *The Combinatorial Index*.

The Combinatorial Index should be an important reference for the veteran practitioner of combinatorial chemistry and will serve as an invaluable tool for the increasing number of researchers that have begun to rely on some element of combinatorial synthesis in their research.

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Theoretical Organic Chemistry. Edited by Cyril Párkányi (Florida Atlantic University). Elsevier: Amsterdam. 1998. xiv + 622 pp. $330.50. ISBN 0-444-82660-2.

This book contains 16 chapters, each written by different authors. The chapters are either reviews of a particular topic or summaries of the authors' work in a particular area. The greatest strength of this book is that the selection of topics gives a good sampling of the breadth and depth of theoretical organic chemistry. Most of the book can be read by someone with an introductory knowledge of theoretical chemistry principles and modeling techniques.

The first chapter of the book (Jan J. C. Mulder) is a historical perspective of the field. This chapter is in places unnecessarily difficult to read because the paragraphs are not indented and it is at times necessary to wade past a litany of researchers' names to find the more important evolution of ideas. The second chapter (Douglas J. Klein) presents a review of valence bond and molecular orbital theories.

Chapter 15 (Branko S. Jursic) gives a good example of how established computational techniques are applied to typical laboratory problems. This is done in the context of Diels−Alder reactions. Chapters 8 and 9 provide more limited examples of the use of established techniques. Chapter 8 (Zvonimir B. Maksić, Mirjana Eckert-Maksić) discusses computed proton activities. Chapter 9 (Cyril Párkányi, Jean-Jacques Aaron) is a discussion of computed dipole moments.

The bulk of this book provides an overview of more recently developed techniques and examples of their usage. Chapter 3 (Tore Brinck) presents an excellent discussion of electrostatic potential analysis. Chapter 4 (Branko S. Jursic) gives a good description of the techniques available to predict reaction selectivity. Chapter 5 (José L. Gázquez) is a discussion of extensions of the concepts of molecular hardness and softness. It contains a large amount of mathematical development, but very few examples of the performance of that theory. Chapter 6 (Tadeusz M. Krygowski, Michal K. Cyrański) is a discussion of information gained from molecular geometry of π-electron compounds. Chapter 7 (Jane S. Murray, Peter Politzer) gives a good discussion of developments in the study of average local ionization energies. Chapter 10 (Dieter Cremer, J. Andreas Larsson, Elfi Kraka) is a discussion of adiabatic vibrational analysis. Chapter 11 (Kenny B. Lipkowitz) presents an excellent review of techniques for modeling enantioselective chromatography retention times, which is currently an industrially important topic. Chapter 14 (László von Szentpály, Ratna Ghosh) is a good review of theoretical and experimental results pertaining to carcinogenicity. Chapter 16 (Martin Klessinger) gives a good discussion of using spin−orbit coupling calculations to predict intersystem crossing in triplet photoreactions.

Chapter 12 (Alexandru T. Balaban) is a review of work done on carbon nets and molecules. It discusses many compounds, but gives only a very minimal description of the work done on each one. Chapter 13 (Davor Juretić, Bono Lučić, Damir Zucić, Nenad Trinajstić) is a discussion of modeling transmembrane protein structures. It summarizes results in this important and timely area; however, there is insufficient discussion of the techniques to be of value to researchers outside that field.

This book goes one step further than being a collection of reviews by having a good selection of topics. Students intending to use theoretical techniques in their future work would benefit from the perspective gained by reading the entire text. Experienced researchers are advised to look over this book in order to avoid the pitfalls of becoming too focused on their own narrow field of research. Overall, the good selection of topics makes this one of the better books available with a review/chapter format.

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