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BOOK REVIEWS

Polyynes: Synthesis, Properties, and Applications. Edited by Franco Cataldo (University of Rome "Tor Vergata", Italy). CRC Press/Taylor and Francis Group. 2006. xviii + 506 pp. $125.96. ISBN 1-57444-512-X.

This book grew out of the proceedings of a 2003 conference in Naples, Italy, called the Interdisciplinary Meeting on Polyynes and Carbyne. Additional scientists were recruited to contribute to the book, helping to round out the selection of material covered. All together, there are 20 chapters, five of which were authored or coauthored by the editor, Franco Cataldo. The strength of this collection is that it captures the full breadth of the field, including bulk and small-molecule synthesis, computational modeling, and studies ranging from astrochemistry and mineralogy to materials science and drug design. This book will be useful to chemists who want to learn more about how other scientists think about polyynes and the putative linear allotrope of carbon, carbyne.

Because so many of the chapters were contributed by the editor, this book has more continuity than many edited volumes. However, there is still a disappointing variation in format, content, and quality of the individual chapters. Many of them, appropriately, review previously published work, with fairly complete bibliographies including references up to 2004. Other chapters, however, have a narrower scope, providing descriptions of new experimental results that do not seem to have been previously presented in the literature. In one chapter, the authors describe a patented material that they call "Tetracarbon", for which they assert many valuable properties, but only cite two papers that they have published in the peer-reviewed literature.

As a result of this diversity, the coverage of the book, while broad, is in some places rather spotty. For example, there is no discussion of the pioneering work from the Tykwinski and Gladysz groups, who have prepared and studied monodisperse linear polyyne compounds containing as many as 28 sp-hybridized carbon atoms. Overall, this book has many interesting and informative sections, which will make it of interest to chemists working with polyynes, but it is not as complete a discussion of the topic as one might wish.

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Electroorganic Reduction Synthesis, Volume 1−2. By Sigeru Torii (Okayama University, Japan). Kodansha, Ltd: Tokyo, and Wiley-VCH Verlag GmbH & Co, KgaA: Weinheim, 2006. xxvi + xxvi + 802 pp. $300.00. ISBN 3-527-31539-X.

The field of synthetic organic electrochemistry is large and growing, which represents a challenge for anyone wishing to enter it, even for those experts who want to keep up with recent developments. This two-volume set should be useful to both groups, as it contains a wealth of information on both practical and mechanistic aspects of organic electrochemical reductions. The author has himself made many contributions to the general area of organic electrochemistry. In this book, he provides good mechanistic discussions on the reduction of alkyl halides, arenes, and activated alkenes, areas I happen to know well, and has chosen examples that give a good overview of each area and should prove useful for those planning further work. Other topics include *inter alia* electroreduction of carbonyl compounds, nitrogen compounds, chalcogens, alcohols, silanes and related group IV compounds, organometallics, indirect electrochemical and electrocatalytic processes, electrogenerated bases, and electropolymerization. The chapter on electrochemical variables such as solvents and electrode materials should be useful, but the few pages devoted to electrochemical cells are too brief to be of use to someone unfamiliar with the area. I would have also liked to have seen a discussion of the value of voltammetry in planning new electrode reactions. Overall, though, the set and the earlier companion volume on electro-oxidations [VCH and Kodansha, 1985] are highly recommended for both practitioners of organic electrochemistry and nonexperts contemplating carrying out an electrosynthesis for the first time.

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Calculation of NMR and EPR Parameters: Theory and Applications. Edited by Martin Kaupp (University of Würzberg), Michael Bühl (Max-Planck-Institute for Coal Research, Mülheim an der Ruhr), and Vladimir G. Malkin (Slovak Academy of Sciences, Bratislava). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2004. xviii + 604 pp. $242.00. ISBN 3-527-30779-6.

Modern studies of molecular structure, conformation, and reactivity rely heavily on magnetic resonance methods that depend on the spin states of either nuclei (NMR) or electrons (EPR). Arguably, NMR has held the limelight, given that it can be applied to virtually any molecular entity in its native, underivatized state. On the other hand, EPR requires the presence of an unpaired spin and, consequently, finds more restricted, albeit important, applications. While experimental magnetic resonance parameters can oftentimes be measured straightforwardly, their interpretation in terms of specific molecular properties can be problematic. For these reasons, considerable effort has been devoted over the past 50 years to developing reliable theoretical methods to predict magnetic resonance parameters using a wide range of computational methodologies. The aims of these calculations are to (a) provide more detailed structural explanations for the origins and magnitudes of the parameters and (b) assist in the treatment and interpretation of experimental data. Indeed, it can be argued that computational methods are essential nowadays for accurate analysis and interpretation of magnetic resonance parameters.

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Parametrization of NMR and EPR parameters, such as chemical shifts, *J*-couplings, and hyperfine coupling constants, cannot be easily accomplished via experimental methods alone, and thus access to accurate methods to calculate them can fill in the gaps in empirical approaches and lead to more reliable structural interpretations.

This book, edited by three well-established investigators in the field of theoretical methods, provides a very broad survey of the current state-of-the-art in the calculation of NMR and EPR parameters. The book is divided into five parts. In Part A, several chapters are devoted mainly to the historical development of the field, from its birth in the mid-20th century to the present. These chapters cover, in general terms, the evolution of the field and how early problems and limitations were systematically addressed by refinement of the theory, development of improved modes of calculation, and advances in computer hardware that rendered more complex, time-consuming accurate treatments practical. Parts B and C are devoted to NMR parameters, with the former focused on methodology and the latter on applications. These two parts take up ca. 60% of the book. Finally, Parts D and E mimic Parts B and C, respectively, as applied to calculations of EPR parameters.

Part B comprises 15 chapters devoted mainly to calculations of NMR chemical shifts and *J*-couplings, as well as quadrupolar couplings. As is true throughout this book, each chapter is modest in length (∼20 pages), so any one treatment is necessarily limited in detail and scope. Several chapters in this section are noteworthy, specifically those devoted to rovibrational corrections by Ruden and Ruud, solvent models by Ciofini, molecular dynamics effects by Searles and Huber, and the interpretation of chemical shifts by Kaupp and *J*-couplings by Malkina. Part C on applications includes eight chapters, and the selection of topics appears somewhat random. For example, topics as diverse as NMR parameters in proteins/nucleic acids by Case to NMR parameters in zeolites by Goursot and Berthomieu to fullerenes by Heine are covered. Given the brevity of these chapters, they are not comprehensive, and readers seeking thorough treatments of these topics may be disappointed. On the other hand, if the reader's aim is to obtain a snapshot of applications in a few diverse fields, the book succeeds nicely.

Part D comprises six chapters that range from DFT calculations of hyperfine coupling tensors by Munzarova to zero-field splittings by Neese. Part E contains two chapters that emphasize some biological applications of EPR parameter calculations.

This book does an admirable job of presenting snapshot pictures of specific topics related to calculations of magnetic resonance parameters. Being an edited text involving more than 45 authors, however, continuity is arguably less than optimal, and it does not treat all active areas of investigation, although perhaps the latter aim would be difficult to achieve in practice. Readers planning to enter the field will find this book an excellent starting point, since each chapter provides a modest list of references for continued study and contains a summary or conclusions section identifying areas where further work is needed. The book treats theory and its evolution very well, and discussions of underlying assumptions and limitations are found throughout. Readers interested in applications will not find this book a core resource unless they have specific interests in the relatively few areas treated.

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