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BOOK REVIEWS

Magnetic Functions beyond the Spin-Hamiltonian. Structure and Bonding, 117. Volume and Series Edited by D. M. P. Mingos (Oxford University, UK). Springer: Berlin, Heidelberg, New York. 2006. x + 276 pp. $325.00. ISBN 3-540-26079-X.

In keeping with the purview of the *Structure and Bonding* series, this volume is a critical review of magnetic functions and the methodologies associated with calculating magnetic parameters, modeling magnetization, and predicting magnetic susceptibility. This topic is particularly timely, as a wide array of emerging technological applications are dependent upon magnetic behavior (including magneto-caloric materials and magneto-optical information storage devices), and spin-based spectroscopy (e.g., ESR) continues to help elucidate biological reaction mechanisms and characterize the structure and bonding of novel compounds. As a brief overview, the volume uses the spin-Hamiltonian formalism to introduce first magnetic parameters (g-factors, the D-parameter, etc.) and then the theoretical formulas necessary to perform energy level calculations of multiterm systems, evaluating the relevant matrix elements including those for electron repulsion, crystal field, spin−orbit interaction, orbital-Zeeman, and spin-Zeeman operators. Examples are limited to mononuclear transition metal d^n complexes.

This review is a highly advanced mathematical treatise that does not dedicate much time to getting a novice in the field up to speed. Detailed appendices augment the readers knowledge; however they should be considered a recap to someone already fluent in the language of mathematics, group theory, and inorganic chemistry. To its benefit, the review collects a great deal of information that is scattered among many texts and is very thorough, clearly presenting functions and details of the theory that are difficult to find elsewhere. I particularly thought that the graphical representations of the magnetic functions complemented the text nicely and was impressed with the completeness of the tables. Although this volume is beyond the scope of the general reader, it is an excellent reference book that will certainly be of use to spectroscopists and theorists alike.

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JA069727Z

10.1021/ja069727z

Bioorganometallics: Biomolecules, Labeling, Medicine. Edited by Gérard Jaouen (Ecole Nationale Supérieure de Chimie de Paris). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim. 2006. xxiii + 444 pp. $170.00. ISBN 3-527-30990-X.

The term "bioorganometallic chemistry" is broadly defined in this text as the chemistry of organometallic complexes relevant to biological processes, as well as chemistry that involves metals attached to biomolecules via metal−carbon linkages. The recent rapid pace of research in this area makes this book a timely overview of progress achieved to date. Jaouen has assembled a group of 16 authors who have produced 12 chapters on a range of topics in this area from ruthenium arene anticancer compounds to organometallic bioprobes to synthetic models for bioorganometallic reaction centers. The vast majority of the citations are from the years 1990 through 2004.

The book achieves the stated objective as a comprehensive review of bioorganometallic chemistry, with only a few exceptions. To be truly comprehensive the text would include a more detailed treatment of vitamin B_{12} and related cobalamin cofactors than that given in the introductory chapter. However, the authors made a conscious decision to limit this coverage due to the well-developed nature of that work. Furthermore, Chapter 11 on metalloenzyme active sites provides an overly broad and superficial review of metal centers found in enzyme active sites, where the organometallic aspect is often either absent or not evident from the presentation.

The quality of most chapters is high, although the chapter on radiopharmaceuticals contains numerous errors in the schemes. This reviewer would have preferred a more specific and detailed discussion of the various biological and medical applications that are often alluded to in the text, although a number of chapters such as that on organometallic complexes as tracers in nonisotopic immunoassay are excellent in this regard.

Overall, this text will serve as an interesting and valuable resource for those who wish to learn more about the progress and challenges that face the immerging field of bioorganometallic chemistry.

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JA0697119

10.1021/ja0697119

Block Copolymers I and II. Advances in Polymer Science 189 and 190. Edited by Volker Abetz (Institut für Polymerforschung, Geesthacht, Germany). Springer: Berlin, Heidelberg, New York. 2005. xx + 238 pp. $199.00. ISBN 3-540-26580-5 (Volume I). xii + 252 pp. $219.00. ISBN 3-540-26902-9 (Volume II).

Block copolymers have been studied for several decades, a period that has been punctuated by a number of books and review articles on the topic. Despite this history, the subject is far from exhausted and, if anything, has experienced a strong renewal in recent years. This has been spearheaded by a vast variety of new block copolymers, the important development of powerful visualization techniques, AFM in particular, that have become readily available, as well as motivating visions of nanotechnological applications.

In this context, this new two-volume book, with its focus on the most recent developments in the area, is timely. It begins with a chapter that summarizes the different synthetic approaches and the various chain architectures that have now been

10.1021/ja069727z CCC: $33.50 © 2006 American Chemical Society

achieved, restricting itself almost exclusively to the period 2000−2004. The length of this chapter, the longest of the five, is illustrative of all the recent activity in the field.

Chapter 1 naturally leads to an update in the following chapter on the morphology of block copolymers and phase behavior in the bulk. The most studied systems in the past have been linear diblocks. Thus, the second chapter emphasizes tri- and multiblock linear copolymers and other architectures, as well as copolymer blends. These have opened the door to a large variety of fascinating new nanostructures and complex phase diagrams. The special case of crystallizable block copolymers is treated in a separate (third) chapter.

Besides the bulk state, there has been enormous interest in block copolymers in the micellar solution state and as thin films. These thus form the subject of two additional chapters (fourth and sixth), with a final one (fifth in order) devoted to investigations of how block copolymers can be manipulated to yield nanoporous materials in both the bulk and as thin films. The promise of block copolymers for useful technologies, running the gamut from stimuli-responsive micelles for medical applications to nanoporous separation membranes to template and nanolithography applications, is particularly evident in these chapters.

Overall, the emphasis is on the “what” and the “how”, rather than the “why”, indicating that a great deal of understanding must still be forthcoming. As a minor point, the reader must overlook some editorial and production errors and some overlap between chapters (including two figures found in both of the last two chapters). These two volumes should be considered indispensable by any newcomer to the subject and will constitute a useful reference for many already in the field.

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JA069709H

10.1021/ja069709h

Intermolecular Forces and Clusters I. Structure and Bonding, 115.

Edited by D. J. Wales (University of Cambridge, UK). Series Edited by D. M. P. Mingos. Springer: Berlin, Heidelberg, New York. 2005. xvi + 206 pp. $199.00. ISBN 3-540-28194-0.

“There’s plenty of room at the bottom.” Richard Feynman in 1960 was referring to the then-nonexistent field of nanoscience, but the statement applies equally well to the weakness and ubiquity of intermolecular forces. Most of the 21 million or so compounds currently registered are molecular in nature, i.e., covalently bonded atomic assemblies. If each of these compounds interacted with another, the intermolecular forces or potential energy surfaces characterizing these interactions would number in the trillions. Thus developing rules for formulating these nonbonded forces between molecules based on whole-molecule, group, or atomic properties is pivotal to delineating the origins of these forces and using them effectively to elucidate and make predictions for polymolecular systems in both chemistry and molecular biology. Like other members of the *Structure and Bonding* series, the present volume is a collection of reviews, here intended to describe the present state-of-the-art in the construction and use of intermolecular force fields. In particular, this is Part I of a two-part collection dedicated to Anthony J. Stone, a pioneer in both high-level ab initio quantum chemistry and the theory and practice of intermolecular forces.

Wales, the editor, has written a very readable introduction, although he apparently did not anticipate the division into two parts: his interweaving of the topics to be presented in both volumes left this reviewer a little wistful for the ones not covered in Part I. As some editors do, he also took the liberty of including a bit on his own research on energy landscapes in large molecules. The topics covered include discussions of quantum chemical topology (QCT), i.e., using the topography of the electron density to define and quantify bonding and forces, by Popelier; angular momentum analysis of ring currents in aromatics by Soncini et al.; the use of intermolecular forces to predict crystal structures by Price and Price; the use of intermolecular forces in molecular dynamics simulations by Millot; and ab initio studies of interactions with aromatics by Tsuzuki. Of these, the analysis of ring currents clearly does not fit with the other topics; although it is quite readable, it looks more like a journal article and has little to do with intermolecular phenomena.

The blue ribbon for best review goes to Price and Price, who taught this reviewer a great deal about the history as well as the current frontier of their field. In particular, they establish the need to go beyond the typical force field that uses atom−atom Lennard−Jones plus partial-charge electrostatics to find potentials that can predict crystal structures and other properties. Certainly the most blood-stirring chapter is Popelier’s lengthy (57 pp) review. His semantic dismantling of Pauling’s definition of a covalent chemical bond left a bad taste—we all know what Pauling *meant* by his statement. At times, Popelier paints QCT as a theory of bonding in competition with valence bond and molecular orbital (MO) methods, although QCT can only commence when presented with a spatial electron distribution $\rho(\mathbf{r})$ derived from one of the other methods. Fiddling with derivatives of ρ in order to locate “bond critical points”, atomic divides, and “bond paths” has been controversial since its inception in the work of Bader’s group. To chemists schooled in the MO approach to molecular structure, trying to find bonds (in the Lewis sense) and atoms in a molecule is hopeless, since the valence electrons as individuals naturally delocalize themselves over the molecular framework. When these ideas are applied to intermolecular interactions, bond critical points appear between any two near-lying nuclei in a polymolecular complex, even though the interaction may be mainly steric repulsion. An area where some useful insight might be had is that of hydrogen bonding; unfortunately Popelier has little enlightening to say on the topographically distinctive features of hydrogen bond electron density, beyond the observation that it is just another bond with a lower electron density at the bond critical point. QCT is having a practical impact on intermolecular forces, which justifies its inclusion in this volume: the partitioning of space into atomistic regions allows for the ready definition of atomic charges and higher multipoles, which has proven useful in constructing accurate electrostatic contributions to intermolecular force fields when carried to sufficiently high order. Popelier’s philosophic ramblings were less informative; in particular, the idea that time has no intrinsic role in defining a quantum system is not new. On the other hand, the review by Millot is a coherent methodological summary of the use of force fields in molecular dynamics, including dynamically changing atomic moments due to induction. Tsuzuki's tables of interaction energies, separated into repulsive, electrostatic, and correlation (translate dispersion) contributions, and energy diagrams were quite enlightening; the emergence of coupled-cluster methods as the "gold standard" for including electron correlation has greatly clarified the nature of X−H/π interactions, which all turn out to have large dispersion terms. Several of the authors have studied with Anthony Stone, and threads of his seminal work show up throughout the volume.

There were the inevitable typographical errors: "polarisabilies", "distorsion", "spurned" instead of "spurred", and "nothing" instead of "noting". The table of contents occurs after a good deal of front matter and the introductory essay, making it a little trouble to locate, and the index is not comprehensive. Overall, however, the literature citations are current, and *Intermolecular Forces and Clusters I* is well-produced. Although it is bit pricey for individual purchase, this volume is a worthy addition to those university chemistry libraries that have a collection in the *Structure and Bonding* series.

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JA059870C

10.1021/ja059870c

Intermolecular Forces and Clusters II. Structure and Bonding, 116. Edited by D. J. Wales (University of Cambridge, UK). Series Edited by D. M. P. Mingos. Springer: Berlin, Heidelberg, New York. 2005. xvi + 158 pp. $175.00. ISBN 3-540-28191-6.

This slim volume, like its predecessor (Volume 115), contains papers written by leading researchers of intermolecular forces and clusters in honor of Anthony Stone. Taken together, the articles provide an accurate snapshot of current work on selected aspects of intermolecular forces and clusters that are primarily, but not exclusively, theoretical. A reader looking for a comprehensive overview of the subject will be disappointed.

Ewing provides a very readable survey of experimental and theoretical work dealing with water on a surface of sodium chloride. His coverage extends from a single water molecule to clusters, monolayers, and thin films. This concise and lucid paper conveys the flavor of the field in a manner that could entice a young student to devote his or her career to intermolecular forces.

Szalewicz, Patkowski, and Jeziorski describe recent theoretical developments in, and applications of, the symmetry-adapted perturbation theory (SAPT) of intermolecular interactions. The first half of the article focuses on the convergence properties of SAPT including some original results and a numerical study of the Li−H interaction. The second half of the article begins with an outline of a new version of SAPT, based on a description of the monomers using density functional theory that can be applied to interactions involving large molecules. This long and insightful article is rounded out by a survey of many recent applications of SAPT, which should give the nonspecialist a good feel for what can and cannot be calculated accurately at this time.

In two other chapters, Xantheas describes his work on developing new, polarizable, interaction potentials for water from accurate calculations on energies of water clusters, and Christie and Jordan detail a new methodology based on *n*-body decomposition that makes second-order Moller−Plesset (MP2) calculations in large basis sets feasible for clusters of as many as 50 water molecules.

Scientists and students interested in pursuing research on intermolecular forces and/or clusters would benefit by reading, or skimming through, this book. This book is strongly recommended for purchase by academic and industrial libraries.

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JA069729J

10.1021/ja069729j