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Book Reviews

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Book Reviews

"Introduction to Theoretical Organic Chemistry and Molecular Modeling" by William B. Smith, VCH Publishers, New York, NY and Weinheim, Germany, 1996; ISBN 1-56081-937-5; xii + 192 pages; $59.95; DM 89.00.

This book arrived in mid-October, 1996 at a time when I was about six weeks into a graduate course "Organic Reaction Mechanisms" that I had not previously taught. I had intended to cover quantum chemistry at a level sufficient to introduce aromaticity and the conservation of orbital symmetry and to introduce the students to molecular mechanics with hands-on access to appropriate software. When I examined this book, its first four chapters (The Hydrogen Atom and the Hydrogen Molecule, Hückel Molecular Orbital Theory, The PMO Method, and Aromaticity, Antiaromaticity, and Resonance) had an eerie similarity to my lecture notes that had been compiled from a variety of sources. Hence, I cannot possibly give this book a weak review! Additional topics covered include FMO and Extended Hückel Theory, orbital symmetry, molecular mechanics, semiempirical SCF-MO methods, and *ab initio* and density functional theory. The first eight of the ten chapters are followed by problem sets for student practice, and references are given at the end of each chapter. An appendix deals with matrices and determinants, especially as applied to obtaining the coefficients of HMOs, and there is an adequate four page index.

The author intends the book to be used by students after a year of physical chemistry, and it is useful for that purpose as well as beginning graduate courses that seek to introduce students to modern theoretical organic chemistry. At appropriate places throughout the book, the author gives meaningful critical appraisal of various software packages. One could argue that much of the material in the middle of the book is now passe, and that it would have been desirable to start with *ab initio* theory and to detail all of the simplifications made until one arrives at HMO theory, but these are perhaps questions of style. I would also have preferred to see more space devoted to Koopmans' theorem and its application via MO methods to the interpretation of photoelectron spectra, and the Born-Oppenheimer approximation should be in Chapter 1.

The book is not without mistakes. The representation of the Claisen rearrangement on p. 83 is an example. Figure 8.1 (p. 119) is not very clear.

The figure on p. 135 is upside down. Mulliken ("Mullikan") is misspelled throughout Chapter 9.

To summarize, the author has assembled a book that will be useful to introduce senior undergraduates, beginning graduate students, and more advanced individuals to the concepts behind the various methodologies presently used in theoretical organic chemistry.

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"**Applications of Organometallic Chemistry in the Preparation and Processing of Advanced Materials**", edited by J. F. Harrod and R. M. Laine, NATO ASI Series E Vol. 297; Kluwer Academic Publishers, Dordrecht, 1995; ISBN 0-7923-3677-1; xii + 355 pages; $183.00; 165 Dfl; 177£.

This book contains the proceedings of the NATO Advanced Research Workshop with the same title held September 4–9, 1994 at Cap D'Agde, France. In addition to three main sections, titled "Metal Oxide Materials-Synthesis, Processing, Characterization", Nonoxide Materials-Synthesis, Processing, and Characterization", and "Novel Materials with Novel Properties", the book contains a list of participants, a list of contributing authors, an author index, and a subject index.

From the preface, the editors note that the common thread for most of the subjects in the book is the synthesis of inorganic objects from organic precursors, and they refer to earlier NATO ASI Workshops on that theme. The section on nonoxide materials deals with polymeric precursors to silicon-containing ceramics. The section on novel materials will be of most interest to readers of this journal. Two chapters deal with polymers containing acetylene groups, two deal with carbon and metal containing cage clusters (fullerenes and "met-cars") and two others deal with assembly methods. Properties of interest include liquid crystalline order (2 chapters), magnetism (2 chapters), and electrical and nonlinear optical properties.

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