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BOOK REVIEWS

Interactions in Molecules: Electronic and Steric Effects. Edited by Sigrid D. Peyerimhoff (Universität Bonn). Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany. 2003. xii + 364 pp. $160.00. ISBN 3-527-27732-3.

This volume is a report on the title topic from those faculties and institutes of the Rheinische Friedrich-Wilhelms-Universität Bonn that comprised the Collaborative Research Center 334 from 1989 to 2000. Their multidisciplinary research on intra- and intermolecular interactions was supported by the Deutsche Forschungsgemeinschaft. The emphasis on chemical design and synthesis, modern spectroscopic experimental methods, and refined algorithms and approaches to quantum mechanical computations is detailed in a 14-page introductory chapter by the editor and in seven diverse specialized chapters. Solving complex problems via the close cooperation of experimental and theoretical efforts is a stimulating and recurrent theme. The longest chapter, nearly one-third of the book, is devoted to the interactions of chiral molecules with circularly polarized light, a difficult research area of great fundamental and practical importance. To improve understanding of the subtle dependence of circular dichroism (CD) on the electronic structure, the researchers working on the project designed and synthesized several very interesting series of kindred chiral molecules based on planar or helical skeletons and differing, for example, by their intramolecular strains. The quantum mechanical computations range from benchmark work on optical rotatory strengths for the simplest chiral system, H_4^{2+}, to work addressing the CD spectra of molecules containing tens of atoms. In some examples, the computations allowed conformers responsible for the observed CD data to be identified with confidence. The importance of producing CD measurements on gaseous samples and including high electronic states is emphasized. The chapter has 157 numbered references, with multiple articles entered under most numbers.

Demonstrating the variety present in this book, there is a chapter devoted to "spin orbit and vibronic coupling effects in open-shell molecules" wherein the measurement and detailed theoretical interpretations of hyperfine structure in the spectra of short-lived radicals as observed using high-resolution laser magnetic resonance (LMR) spectroscopy are discussed. The transmutation of the original LMR experimental method into the Faraday LMR spectroscopy method used in their work is described. There is an extensive discussion of effective Hamiltonians and the procedures used for the quantum mechanical computation of the intricate electronic coupling behaviors. Detailed results are presented for more than a dozen specific diatomic (e.g., NiH and NiD), tetra-atomic (e.g., HCCO), and triatomic molecules. The latter group includes C_2H (ethyinyl radical), which is presented by the authors as perhaps foremost among exemplars currently requiring both experimental and theoretical input for satisfactory understanding.

Space limitations allow only cursory mention of the five other chapters. One of these is a description of work on the interactions of atomic core electrons with the valence shell through the study of X-ray absorption near edge structures (XANES) and Auger spectra, with theory and computation devoted to the relevant electronic excitation and decay processes. The P_4O_6 and P_4O_6X (X = O, S, Se) family is important among the subject molecules, and comparative behavior of effects due to their electronic structures, this time as reflected by vibrational spectroscopy, is presented in a separate chapter. Weakly interacting complexes are addressed in a theoretically oriented chapter, with the extensive spectroscopic results obtained for Ar·CO treated explicitly. There is also a chapter divided between sections devoted to CO or other molecules adsorbed on binary metal alloy surfaces and to UV spectroscopic studies of NH and ND isolated in rare gas solids. Another chapter, "Interactions in Transition Metal Chemistry and Catalysis", is also split between two topics. The parahydrogen-induced polarization (PHIP) effect in NMR spectroscopy, which arises in spectra for reactions involving the addition of *para*-hydrogen diatoms to double bonds, is the subject of the first section. PHIP methods allow mechanisms and rates of the reactions to be investigated, with frequent detection of transient reaction intermediates. A detailed discussion of the chromium-mediated benzannulation reaction is presented in the second section.

Separate bibliographies accompany each chapter. Most of them are extensive, and they naturally favor publications originating from the Cooperative Research Center 334. Unfortunately, there is no author or subject index. I found this book-length summary of the results of 11 years of intensive multidisciplinary research stimulating and certainly worth the time spent reading it. It is well-written and referenced and broad in scope, and it unfailingly held the attention of this physical chemist.

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