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BOOK REVIEWS

Non-Covalent Interactions: Theory and Experiment. By Pavel Hobza (Academy of Sciences of the Czech Republic, Prague, Czech Republic) and Klaus Müller-Dethlefs (University of Manchester, U.K.). Royal Society of Chemistry: Cambridge. 2010. xii + 226 pp. $159. ISBN 978-1-84755-853-4.

The authors of *Non-Covalent Interactions: Theory and Experiment* have undertaken an extremely daunting task and produced what will undoubtedly be a welcome addition to bookshelves already populated with texts dedicated to hydrogen bonding, dispersion forces, and the like. Recognizing that these interactions are so ubiquitous that no single text can hope to provide a thorough overview of the subject, the authors have struck a fine balance between what is possible and what is feasible. Readers should not expect this 226-page book to provide a comprehensive review or exhaustive summary of the literature but instead can look forward to perspectives and insight from two of the world's foremost experts in the field.

In this book, Hobza and Müller-Dethlefs present a good overview of many of the theoretical and experimental considerations important to the study of the entire spectrum of non-covalent interactions. They discuss a number of examples from the literature and provide the reader with an excellent commentary on each. Despite their focus on gas-phase interactions due to their desire to compare experiment and theory directly, they develop concepts that are also applicable to the condensed phases. Although portions of the text could serve as introductory material to advanced undergraduates, it is most appropriate for those with some research experience in the field, particularly a graduate level audience that is already familiar with the fundamentals of quantum chemistry.

The authors begin with a detailed introduction to the subject of non-covalent interactions with an emphasis on nomenclature and definitions of what constitutes the different types of interactions. They discuss the important contributions of non-covalent interactions in nature that will be built upon in later chapters and also introduce many of the experimental and theoretical methods employed for the study of these interactions. Chapter 2 introduces many of the observables that experimentalists attempt to measure and theoretical chemists attempt to predict. These include comparing experimental and theoretical vibrational frequencies, relating average geometry to potential energy surfaces, and determining the stabilization energy of two or more weakly interacting species.

The next chapter is a rather lengthy discussion of potential-energy and free-energy surfaces. The authors start with a detailed description of the archetypal benzene dimer system, which is the model system for discussing weak, non-covalent π-type interactions. This system has served for years as the prototype for discussing interactions between delocalized electron systems in biology. The remainder of this chapter is dedicated to a myriad of theoretical studies from the literature involving weakly interacting benzene analogues, such as amino acids, nucleic acid−base pairs, and microhydrated biological building blocks.

In Chapter 4, the authors straightforwardly discuss the types of non-covalent complexes as determined by the dominant contributor to the stabilization energy. They include a comparison of hydrogen bonding to improper hydrogen bonding. The following two chapters conclude the text with a review of a number of previous experimental studies of weakly bound clusters and their analyses using high-level computations. A good variety of experimental methods employed to study neutral molecular clusters are covered in Chapter 5, including MATI, ZEKE, and R2PI. Chapter 6 includes discussions of protonated water clusters, aerosols, and chiral recognition but no references to negatively charged molecular clusters, such as those incorporating a solvated electron (with ammonia or water, for instance), dipole-bound electrons, or anions. Also absent are the more strongly bound molecular clusters incorporating positively charged metal atoms.

Co-authorship by an eminent theoretician and an eminent experimentalist is certainly a unique feature of the book. Readers will gain appreciation for the difficulties of establishing a connection between the two areas for non-covalent interactions. The book also addresses the entire spectrum of non-covalent interactions, not just one specific type, e.g., hydrogen bonding. Although the authors tend to focus on systems ranging from two to several dozen atoms, the vast majority of material presented in this book is applicable to both larger and smaller systems. The references are somewhat selective, but this personal bias tends to be offset by surprisingly up-to-date citations for a book (as recent as 2009). Overall, we find this monograph to be a valuable resource that will be required reading for graduate students in our laboratories for years to come.

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