Additions and Corrections

Charge-Shift Bonding in Group IVB Halides: A Valence Bond Study of MH_3-Cl (M = C, Si, Ge, Sn, Pb) Molecules [*J. Am. Chem. Soc.* **1999**, *121*, 822]. AVITAL SHURKI, PHILIPPE C. HIBERTY, AND SASON SHAIK*

Table 2: The D_e value in entry 5a for M = C should be 80.2 kcal/mol.

Table 5: The first RE_{cs} value for Sn should be 46.0 kcal/mol. The RE_{cs} values for Pb should be 44.1, 52.0, and 47.5 kcal/mol from top to bottom in the column. The trends and discussions are not affected by the changes in these values.

Table 6: The $D_{3\times3}$ value (at the SD-BOVB level) for H_3Si-Cl should be 102.1 kcal/mol. Footnote *b* to the Table should read as follows: [b] The bonding energy due to all three VB structures **1**, **2**, and **3**. The values are determined at the SD-BOVB geometries.

Reference 52: Schreiner, P. R. should be added as the last name in the list of Editors.

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Book Reviews

Intermolecular Interactions. Edited by Werner Gans (Free University of Berlin) and Jan C. A. Boeyens (University of the Witwatersrand). Plenum Press: New York. 1998. 164 pp. $95.00. ISBN 0-306-45922-1.

This book contains the proceedings of the Second Structural Chemistry Indaba on Intermolecular Interactions, which took place in Kruger Park, South Africa, in August 1997. A short introductory essay by Sommerer describes the purpose of the book, and the meeting upon which it was based, as an attempt by scientists of diverse backgrounds to examine the fundamental concepts related to the interaction of molecules with their environments. Sommerer also raises one of the central questions addressed by many of the other authors, namely, "What exactly constitutes a molecule?" The remaining 12 contributions can be broadly grouped into theoretical, experimental, and data mining approaches to this problem.

In a thought-provoking essay, Boeyens expands on the question of what defines a molecule by developing an alternative qualitative picture of all chemical interactions as a continuum, beginning with the weakest intermolecular interactions and ending with the covalent bond. The next two papers examine the limitations of traditional quantum mechanics for describing the interaction of a molecule with its surroundings. Amman presents a detailed development of how stochastic dynamics may be included into standard quantum mechanics. He also shows how this combined formalism may be used both to describe the behavior of single quantum systems and to reinterpret the behavior of ensembles. In his contribution, Sutcliffe develops a framework for quantum mechanical description of a single molecule in a field or a collection of molecules. Ogilvie bridges the worlds of theory and experiment with an informative primer on the dynamics of intermolecular interactions, in both the gas and the condensed phases.

The measurement of electron density (ED) and the use of the resulting data are the subject of two essays. Koritsánskzy explores the application of ED studies for the characterization of intermolecular interactions such as hydrogen bonding, while Krüger et al. examine its use for explaining reactivity in the solid state. These two contributions combine to serve as a useful introduction to both the methodology of ED studies and the interpretation of the results. Comba provides a careful study of how subtle nonbonding interactions can influence the physical behavior of transition metal complexes; this essay also includes a brief but important discussion of the assumptions implicit in using force fields for molecular modeling. Two essays that are somewhat disconnected from the central theme of the book are those of Bernal et al. and Benson and Cundari. The former contribution presents a study on the crystallization of hydronium salts of metal amine carboxylate complexes, while the latter examines cyclometalation reactions of alkylphosphines.

The three data mining papers included in the volume present a very good introduction to this type of structural analysis. Braga and Grepioni use an observational approach to demonstrate the ubiquitous nature of C−H···O hydrogen bonding in organometallic substances and its central role in determining the supramolecular structure of these substances. Osawa et al. discuss the use of genetic algorithms for determining crystal structures and examine the validity of the van der Waals parameters which are included in modern force field programs. Using statistical analysis, Allen shows how systematic knowledge about noncovalent interactions can be extracted from the Cambridge Structural Database. He also discusses how this information can be augmented with ab initio calculations.

On the whole, the individual essays in this book are generally well-written and include substantial current references. Furthermore, with the exceptions noted above, the essays blend together well to create a comprehensive and intellectually stimulating overview of the nature of chemical interactions in the broadest sense. As such, this book should appeal to anyone interested in how molecules interact with each other or their environments.

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