BOOK REVIEWS

Z. B. Maksić and W. J. Orwille-Thomas, Ed's. Pauling's Legacy, Modern Modeling of Chemical Bond, Theoretical and Computational Chemistry, Vol. 6.

Elsevier Science, Amsterdam, 1999.

This 6th volume in the series of the Elsevier books on new trends in theoretical, notably, computational, chemistry is guite appropriately entitled Pauling's Legacy, because it affords both new progress in chemical conceptualism and applications of computational chemistry to the studies of large molecules and supramolecular structures. It consists of 28 chapters (review articles), on 755 pages, written by recognized authors. Chapters focused on some basic chemical concepts, such as problems of Born-Oppenheimer approximation, definitions of chemical structure or electronegativity, aromaticity and Mills-Nixon effect etc. demonstrate the modern development of theoretical models which were more or less established already in Pauling's work. As many as five chapters deal with the VB theory, reexamining its fundamental methodology and extent by representing its lastest progress and applications. Few reviews are focused on more specialized fields, such as explosions and energetic compounds, polarizability and hyperpolarizability, hydrogen bonds, predicting structures of compounds in the solid state, intermetallic compounds, and three-electron chemical bonding.

Almost half of the book involves an overview of new approaches to the investigations of the »quasicovalent« or noncovalent interactions, which are extremely important in host-guest chemistry. The chapter on the silyl cation problem investigates these interactions at the most fundamental level, but there are also reviews that discuss Van der Waals bonds and interactions in protein molecules. The latest research in the methods of calculations used in the estimation of charge distribution and the shape of large molecules is also presented.

This volume is a highly informative outstanding text not only for researches but also for advanced students.

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