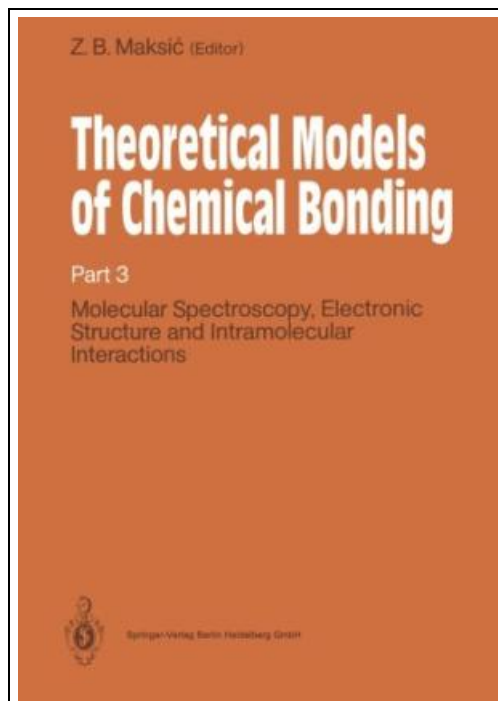


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THEORETICAL MODELS OF CHEMICAL BONDING



Book Condition: New. Publisher/Verlag: Springer, Berlin | Part 3: Molecular Spectroscopy, Electronic Structure and Intramolecular Interactions | The renowned theoretical physicist Victor F. Weisskopf rightly pointed out that a real understanding of natural phenomena implies a clear distinction between the essential and the peripheral. Only when we reach such an understanding - that is to say when we are able to separate the relevant from the irrelevant, will the phenomena no longer appear complex, but intellectually transparent. This statement, which is generally valid, reflects the very essence of modelling in the quantum theory of matter, on the molecular level in particular. Indeed, without theoretical models one would be swamped by too many details embodied in intricate accurate molecular wavefunctions. Further, physically justified simplifications enable studies of the otherwise intractable systems and/or phenomena. Finally, a lack of appropriate models would leave myriads of raw experimental data totally unrelated and incomprehensible. The present series of books dwells on the most important models of chemical bonding and on the variety of its manifestations. In this volume the electronic structure and properties of molecules are considered in depth. Particular attention is focused on the nature of intramolecular interactions which in turn are revealed by various types of molecular spectroscopy. Emphasis is put on the conceptual and interpretive aspects of the theory in line with the general philosophy adopted in the series. | Nuclear Vibrations and Force Constants.- Some Aspects of the Quantumchemical Interpretation of Integrated Intensities of Infrared Absorption Bands.- The Orbital Concept as a Foundation for Photoelectron Spectroscopy.- The Equivalent Bond Orbital Model and the Interpretation of PE Spectra.- Through-space and Through-bond Interactions as Mirrored in Photoelectron Spectra.- Penning Ionization The Outer Shape of Molecules.- The Meaning and Distribution of Atomic Charges in Molecules.- Electron Spectroscopy for Chemical Analysis (ESCA) Basic Features and Their Model Description.-...



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