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ContentsPrefaceI Introduction 1.1 The Basic Postulates of Quantum Mechanics 1.2 Hamiltonian Operators 1.3 Theories of Chemical Bonding Problems References Supplementary Reading II Huckel Molecular Orbital Theory II.1 Basic Assumptions II.2 The Variation Principle II.3 The Basic Hückel Method II.4 Application of the HMO Method to Simple II-Systems II.5 Calculation of the MO Coefficients II.6 Bond Orders and Electron Densities II.7 Alternant and Nonalternant Hydrocarbons Problems References Supplementary Reading III The Use of Symmetry Properties in Simplifying HMO Calculations III.1 Application of Elementary Group Theory III.2 Use of Symmetry to Simplify Secular Determinants Problems References Supplementary Reading IV Polyene Stabilities, Hückel's Rule, and Aromatic Character IV.1 Acyclic and Cyclic Polyenes IV.2 Even- and Odd-Numbered Linear Polyenes IV.3 Linear and Branched Chain Polyenes IV.4 Cyclic Systems Containing (4n + 2) π -Electrons IV.5 Hückel's Rule and the Annulenes IV.6 Polycyclic Systems Problems References Supplementary Reading V Extensions and Improvements of the Simple Hückel Method V.1 Systems Involving Heteroatoms V.2 Inclusion of Differential Overlap V.3 Self-Consistent HMO Methods V.4 The Extended Hückel(EHMO) Method Problems References Supplementary Reading VI The Quantitative Significance of HMO Results The Relationship of HMO Results to Molecular Properties Conclusion Problems References Supplementary Reading VII The Principle of Conservation of Orbital Symmetry VII. 1 Selection Rules for Intramolecular Cycloadditions VII.2 The Woodward-Hoffmann Rules Diagrams VII.3 Energy Level Correlation VII.4 State-Correlation Diagrams VII. 5 Intermolecular Cycloadditions VII.6 Sigmatropic Reactions VII.7 Generalized Selection Rules for Pericyclic Reactions Problems References Supplementary Reading VIII The Möbius -Hückel concept VIII. 1 Hückel Systems VIII.2 Möbius Systems VIII.3 Application of the Möbius-Hückel Differentiation to Concerted Reactions Problems References Supplementary ReadingIX Symmetry, Topology, and Aromaticity IX.1 Aromaticity for Pericyclic and Other Topologies IX.2 HMO Calculations on Nonplanar Systems IX.3 Orbital Interaction Diagrams IX.4 MO Following Problems References Supplementary Reading INDEX Valence bond (VB) theory gave us a qualitative picture of chemical bonding, which was useful for predicting the shapes of molecules, bond strengths, etc. It fails to describe some bonding situations accurately because it ignores the wave nature of the electrons. Molecular orbital (MO) theory has the potential to be more quantitative. With it we can also get a picture of where the electrons are in the molecule, as shown in the image at the right. This can help us understand patterns of bonding and reactivity that are otherwise difficult to explain. Although MO theory in principle gives us a way to calculate the energies and wavefunctions of electrons in molecules very precisely, usually we settle for simplified models here too. These simple models do not give very accurate orbital and bond energies, but they do explain concepts such as resonance (e.g., in the ferrocene molecule) that are hard to represent otherwise. We can get more accurate energies from MO theory by computational "number crunching." While MO theory is more correct than VB theory and can be very accurate in predicting the properties of molecules, it is also rather complicated even for fairly simple molecules. For example, you should have no trouble drawing the VB pictures for CO, NH3, and benzene, but we will find that these are increasingly challenging with MO theory. The lowest unoccupied molecular orbital of the carbon monoxide molecule is a π antibonding orbital that derives from the 2p orbitals of carbon (left) and oxygen (right) Warren J. Hehre is the author of AB INITIO Molecular Orbital Theory, published by Wiley. Leo Radom, born on December 13, 1944 in Shanghai, China, is a computational chemist. He attended North Sydney Boys High School. He has a PhD and a DSc from the University of Sydney and carried out post-doctoral work under the late Sir John Pople. Skip to main search results Hardcover. Condition: Good. Connecting readers with great books since 1972! Used textbooks may not include companion materials such as access codes, etc. May have some wear or writing/highlighting. We ship orders daily and Customer Service is our top priority!. 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