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Nota di contenuto	CONTENTS; PREFACE; 1 SYMMETRY AND STEREOCHEMISTRY; Purpose; Definition of a Group; Molecular Point Groups; Schoenflies Notation; Interrelations of Symmetry Elements; Type Classification; Isomerism and Measurements; Stereoisomerism of Molecules; Stereotopic Relationships of Groups in Molecules; Asymmetric Synthesis and Stereochemistry; NMR and Stereochemistry; Symmetry and Structural Parameters; Note on Hybridization; Symmetry and Orbitals; Atomic Orbitals; Molecular and Group Orbitals; In What Combination?; 2 MOLECULAR ORBITAL THEORY; Introduction; Electronic Schrodinger Equation (A.1) Fock Equations (A.42)The Basis Set (STO-3G, 6-31G*, and All That); Orbital Energies and Orbitals; Representation of MOs; Total Energies and the Hartree-Fock Limit; Successes and Failures of Hartree-Fock Theory; Beyond Hartree-Fock; Density Functional Theory; Geometry Optimization; Normal Coordinates and Harmonic Frequency Analysis; Zero Point Vibrational Energies; 3 ORBITAL INTERACTION THEORY; Relationship to Hartree-Fock Equations; Huckel Approximation; Orbital

Energies and Total Electronic Energy; Case Study of a Two-Orbital Interaction; Case 1: [sub(A)] = [sub(B)], S[sub(AB)] = 0
Case 2: [sub(A)] = [sub(B)], [sub(AB)] > 0, [sub(AB)] « 1Case 3: [sub (A)] > [sub(B)], S[sub(AB)] = 0; Case 4: [sub(A)] > [sub(B)], S[sup(AB)] > 0; Effect of Overlap; Energetic Effect of Overlap; Orbital Effect of Overlap; First Look at Bonding; Relationship to Perturbation Theory; Generalizations for Intermolecular Interactions; Energy and Charge Distribution Changes from Orbital Interaction; Four-Electron, Two-Orbital Interaction; Three-Electron, Two-Orbital Interaction; Two-Electron, Two-Orbital Interaction; One-Electron, Two-Orbital Interaction; Zero-Electron, Two-Orbital Interaction
Interactions between Molecules: Many Electrons, Many OrbitalsGeneral Principles Governing the Magnitude of h[sub(AB)] and S[sub(AB)]; Interactions of MOs; Electrostatic Effects; Group Orbitals; Zero-Coordinated Atoms; Monocoordinated Atoms; Dicoordinated Atoms; Tricoordinated Atoms; Tetracoordinated Atoms; Assumptions for Application of Qualitative MO Theory; Example: Carbonyl Group; Construction of Interaction Diagram; Interpretation of Interaction Diagram; Chemical Reactivity; Why Does It Work and When Might it Not?; 4 SIGMA BONDS AND ORBITAL INTERACTION THEORY
C-X Bonds: X = C, N, O, F and X = F, Cl, Br, I Bonds: Homolytic versus Heterolytic Cleavage; Heterolytic Cleavage of Bonds Involving C or H; Homolytic Cleavage of Bonds Involving C or H; Homonuclear Bonds C-C, N-N, O-O, F-F, Cl-Cl, Br-Br, and I-I; Interactions of Bonds; Bonds as Electron Donors or Acceptors; Bonds as Electron Acceptors; As a Acceptor; As a Acceptor; Bonds as Electron Donors; As a Donor; As a Donor; Bonding in Cyclopropane; 5 SIMPLE HUCKEL MOLECULAR ORBITAL THEORY; Simple Huckel Assumptions
Charge and Bond Order in SHMO Theory: (S[sub(AB)] = 0, One Orbital per Atom)

Sommario/riassunto

A practical introduction to orbital interaction theory and its applications in modern organic chemistry Orbital interaction theory is a conceptual construct that lies at the very heart of modern organic chemistry. Comprising a comprehensive set of principles for explaining chemical reactivity, orbital interaction theory originates in a rigorous theory of electronic structure that also provides the basis for the powerful computational models and techniques with which chemists seek to describe and exploit the structures and thermodynamic and kinetic stabilities of molecules. Orbital Interaction