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Autore	Rauk Arvi <1942->
Titolo	Orbital interaction theory of organic chemistry [[electronic resource] /] / by Arvi Rauk
Pubbl/distr/stampa	New York, : Wiley-Interscience, 2001
ISBN	1-280-26470-5 9786610264704 0-470-35106-3 0-471-46184-9 0-471-22041-8
Edizione	[2nd ed.]
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Disciplina	547.128 547/.128
Soggetti	Molecular orbitals Physical organic chemistry Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	"A Wiley-Interscience publication."
Nota di bibliografia	Includes bibliographical references (p. 313-324) and index.
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

2. Record Nr. UNINA9910482958103321

Autore	Manutchehr-Danai Mohsen
Titolo	Dictionary of Gems and Gemology [[electronic resource] /] / by Mohsen Manutchehr-Danai
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ISBN	3-540-72816-3
Edizione	[3rd ed. 2009.]
Descrizione fisica	1 online resource (1500 illus. eReference.)
Collana	Springer reference
Altri autori (Persone)	WitschelChristian <1966-> KindlerKerstin
Disciplina	553.803
Soggetti	Mineralogy Geology Mineral resources Mineral Resources
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Editors from t.p. verso.
Nota di bibliografia	Includes bibliographical references and index.
Sommario/riassunto	The rapid growth of gemological sciences and mineralogy requires a comprehensive dictionary for gemologists, mineralogists, geologists, jewel dealers, industry, and hobbyists. The third edition of this dictionary contains about 24,000 entries – about 4,000 more than the second edition. The comprehensive definitions are now completed by more than 1,500 charts, diagrams and figures. The author offers a one-stop reference to any matter dealing with gems and gemology. Review of the 1st edition, published in the March 2001 issue of CHOICE “Detailed and highly technical, this work provides encyclopedic coverage of terms, techniques, places, and people related to gems and gemology. Each entry includes scientific and historical information, often illuminated by a line drawing. The volume’s strength lies in its comprehensive scope; it treats all aspects of gemology beginning with the gems themselves, elaborates on technical methods and procedures, explicates professional terminology, and identifies individuals and associated groups. Supplementing the text, 21 tables contain such relevant information as atomic weights, light spectrum, and geological

timetables. Given its useful format and comprehensiveness, the book will serve as an invaluable reference source for practitioners and serious scholars in the field.” L. Doumato, National Gallery of Art.