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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: $[E_A] = [E_B]$, $S_{AB} = 0$
 Case 2: $[E_A] = [E_B]$, $[E_{AB}] > 0$, $[E_{AB}] \ll 1$ Case 3: $[E_A] > [E_B]$, $S_{AB} = 0$; Case 4: $[E_A] > [E_B]$, $[E_{AB}] > 0$; 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 Orbitals
 General Principles Governing the Magnitude of H_{AB} and S_{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: ($S_{AB} = 0$, 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

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Anderson, Dean Smith, Hazel Woodward, Allen Renear. -- Charleston Conference observatory: are social media impacting in research? / David Nicholas, Ian Rowlands, Deanna Wamae. -- The tower and the free web--the role of reference / John Dove, Phoebe Ayers, Casper Grathwohl, Jason B. Phillips, Michael Sweet. -- Full-spectrum stewardship of the record of scholarly and scientific research / Brian E. C. Schottlaender. -- Executives' roundtable / T. Scott Plutchak, Youngsuk (YS) Chi, Kent Anderson. -- When rubber meets the road: rethinking your library collections / Roger Schonfeld, Sue Woodson. -- What can our readers teach us? / John Sack. -- "I hear the train a comin'" -- LIVE / Greg Tananbaum, Joseph J. Esposito. -- Creating a trillion-field catalog: metadata in Google Books / Jon Orwant. -- Efficient and effective funding of open access 'books' / Frances Pinter. -- The long arm of the law / Ann Okerson, William Hannay, Lauren K. Schoenthaler. -- E-everything, putting it all together / Peter McCracken. -- Innovative practices in electronic resources and acquisition management / Ryan Weir, Geoffrey P. Timms, Kelly A. Smith, Regina Koury, Denise Pan. -- What do those collection numbers in resources for college libraries really mean? / Susan K. Beidler. -- What's in your aggregator?: context, currency, and stability of full-text databases / Mary Beth Chambers, Mariyam Thohira, Nancy Sprague. -- Taking a step back, to move forward / Stephen Dew, Michael Crumpton. -- Collection intelligence: using data driven decision making in collection management / Annette Day, Hilary Davis. -- Disaster mental health: building a research level collection / Ardis Hanson, Claudia J. Dold. -- From monks to mutopia: changing landscape in sheet music publishing / Ana Dubnjakovic. -- Deselecting the monographs collection: one library's adventure in weeding / Margaret Foote, Betina Gardner. -- OARS: toward automating the ongoing subscription review / Geoffrey P. Timms, Jonathan H. Harwell. -- Wherefore are thou, RoMEO? -- a review of open access-public access definitions and policies / Betty Landesman. -- Consensus-based assessment for re-envisioning a reference collection / Michael A. Matos, Patricia J. West. -- Moving from print to electronic journals: a study of college and university libraries in Indiana / Jo McClamroch. -- Weeding with robots: managing collections in an automated retrieval system / Patricia Bravender, Robert Kelly, Linda Masselink, Hazel McClure. -- Looking forward by looking back: books at the end of the book / Darby Orcutt, Genya O'Gara. -- The GIST gifts & de-selection manager: redesigning gift and weeding workflow in the library / Kate Pitcher. -- Chinese scientific journals: an assessment of the need at Cornell / Jinxia Huang, Marty Schlabach. -- Patron driven acquisitions: the future of collection development? / Rebecca Schroeder, Tom Wright, Robert Murdoch. -- How to evaluate cultural authenticity and stereotypical generalizations that exist in Asian-American children's books / Tadayuki Suzuki. -- Changes in print paper during the 19th century / AJ Valente. -- The other side of the coin: de-selecting material from a research library's storage facility / Suzanne M. Ward. -- Issues in determining cost for cost per use calculations / Virginia Kay "Ginger" Williams. -- Core resources on time series analysis for academic libraries: a selected, annotated bibliography / Sarah H. Jeong. -- Using DASH! for digital repositories: a case study of the East Texas Baptist University Library / Cynthia L. Peterson. -- Library connections: a non-linear approach to planning, marketing and creating the positive user experience / Leah M. Dunn. -- E-paper, LED, OLED, and the strategic positioning of hardware vendors and publishers: what it means to libraries / Stephen Patton. -- From my library to our library: changing a culture in tough times / Robert Alan, Lisa German. -- The "Get It" department: Oregon State University's

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Sommario/riassunto

The Charleston Conference Proceedings documents one of the most highly regarded and influential conferences in the international library world. This volume marks and celebrates the 30th Annual Charleston Conference. The 2010 Conference focused on topics and trends in: • Collection Development • Journals and Serials Management • Technology and Product Development • Collaboration between and among Libraries and their Communities • Managing eBook and Monograph Collections
