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Nota di contenuto	ELECTRONIC STRUCTURE AND PROPERTIES OF TRANSITION METAL COMPOUNDS; CONTENTS; Preface; Foreword to the First Edition; Mathematical Symbols; Abbreviations; 1 Introduction: Subject and Methods; 1.1 Objectives; Molecular Engineering and Intuitive Guesswork; Main Objectives of This Book in Comparison with Other Sources; 1.2 Definitions of Chemical Bonding and Transition Metal Coordination System; Chemical Bonding as an Electronic Phenomenon; Definition of Coordination System; 1.3 The Schrodinger Equation; Formulation; Role of Approximations; Summary Notes; References; 2 Atomic States 2.1 One-Electron StatesAngular and Radial Functions; Orbital Overlaps: Hybridized Functions; Spin-Orbital Interaction; Relativistic Atomic Functions; 2.2 Multielectron States: Energy Terms; Electronic Configurations and Terms; Multielectron Wavefunctions; Slater-Condon and Racah Parameters; The Hartree-Fock Method; Summary Notes; Questions; Exercises and Problems; References; 3 Symmetry Ideas and

Group-Theoretical Description; 3.1 Symmetry Transformations and Matrices; 3.2 Groups of Symmetry Transformations; Example 3.1. The Symmetry Group of an Octahedral O(h) System and Its Classes 3.3 Representations of Groups and Matrices of Representations3.4 Classification of Molecular Terms and Vibrations, Selection Rules, and Wigner-Eckart Theorem; Example 3.2. Energy Terms of Electronic Configuration e(2); 3.5 Construction of Symmetrized Molecular Orbitals and Normal Vibrations; Example 3.3. Construction of E(g)-Symmetry-Adapted MOs for Octahedral O(h) Systems; Example 3.4. Construction of T(2g)-Symmetry-Adapted MOs for Octahedral O(h) Systems; Example 3.5. Normal Coordinates of a Regular Triangular Molecule X (3); 3.6 The Notion of Double Groups; Summary Notes; Exercises References4 Crystal Field Theory; 4.1 Introduction; Brief History; Main Assumptions; 4.2 Splitting of the Energy Levels of One d Electron in Ligand Fields; Qualitative Aspects and Visual Interpretation; Calculation of the Splitting Magnitude; Example 4.1. Splitting of a d-Electron Term in Octahedral Crystal Fields; Group-Theoretical Analysis; 4.3 Several d Electrons; Case of a Weak Field; Strong Crystal Fields and Low- and High-Spin Complexes; Example 4.2. High- and Low-Spin Octahedral Complexes of Iron; Energy Terms of Strong-Field Configurations Example 5.1. Shortcomings of Mulliken's Definition of Atomic Charges in Molecules

Sommario/riassunto

With more than 40% new and revised materials, this second edition offers researchers and students in the field a comprehensive understanding of fundamental molecular properties amidst cutting-edge applications. Including ~70 Example-Boxes and summary notes, questions, exercises, problem sets, and illustrations in each chapter, this publication is also suitable for use as a textbook for advanced undergraduate and graduate students. Novel material is introduced in description of multi-orbital chemical bonding, spectroscopic and magnetic properties, methods of electronic structure calculation, an