1. Record Nr. UNISA990000564800203316

Titolo	3: Il differenziamento / a cura di Giulio Lanzavecchia
Pubbl/distr/stampa	Milano : Le Scienze S.p.A., 1980
ISBN	88-7004-044-5
Descrizione fisica	167 p. : ill. ; 29 cm
Collana	Letture da Le Scienze ; 20
Disciplina	574.8
Collocazione	500 SC 20/III Coll.AUH 7/3
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia

2. Record Nr. UNINA9911019652203321

Autore	Bersuker I. B (Isaak Borisovich)
Titolo	Electronic structure and properties of transition metal compounds : introduction to the theory / / Isaac B. Bersuker
Pubbl/distr/stampa	New York, : Wiley, c2010
ISBN	9786612684708 9780470920855 0470920858 9781282684706 1282684701 9780470573051 0470573058 9780470573044 047057304X
Edizione	[2nd ed.]
Descrizione fisica	1 online resource (797 p.)
Collana	Textbook for graduate and advanced undergraduate students
Disciplina	546/.6
Soggetti	Transition metal compounds Chemistry
Lingua di pubblicazione	Inglese

Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
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