1. Record Nr. UNISA996214586503316

Titolo	The journal of biophysical and biochemical cytology
Pubbl/distr/stampa	New York, N.Y., : Rockefeller Institute for Medical Research, 1955-1961
ISSN	2327-7440
Disciplina	574
Soggetti	Cytology Biophysics Biochemistry Cells cells Periodical Periodicals.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Periodico
Note generali	Title from cover (JSTOR, viewed Mar. 8, 2006). Published by: Rockefeller Institute, 1958-July 1960; Rockefeller Institute Press, Sept. 1960-Dec. 1961.

2. Record Nr. UNICAMPANIAVAN00006514

Titolo	Dalla rivoluzione bolscevica alla Federazione russa : traduzione e commento dei primi atti normativi e dei testi costituzionali / [a cura di] Giovanni Codevilla
Pubbl/distr/stampa	Milano, : Angeli, [1996]
Descrizione fisica	541 p. ; 22 cm.
Disciplina	342.47023
Soggetti	Russia - Costituzioni politiche - 1993 Unione Sovietica - Costituzioni politiche
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia

3. Record Nr. UNINA9910813258303321

Autore	Shaik Sason S. <1943->
Titolo	A chemist's guide to valence bond theory / / Sason Shaik, Philippe C. Hiberty
Pubbl/distr/stampa	Hoboken, N.J., : Wiley-Interscience, c2008
ISBN	9786611134853 9781281134851 1281134856 9780470192597 0470192593 9780470192580 0470192585
Edizione	[1st ed.]
Descrizione fisica	1 online resource (332 p.)
Altri autori (Persone)	HibertyPhilippe C
Disciplina	541/.224
Soggetti	Valence (Theoretical 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	A CHEMIST'S GUIDE TO VALENCE BOND THEORY; CONTENTS; PREFACE; 1 A Brief Story of Valence Bond Theory, Its Rivalry with Molecular Orbital Theory, Its Demise, and Resurgence; 1.1 Roots of VB Theory; 1.2 Origins of MO Theory and the Roots of VB-MO Rivalry; 1.3 One Theory is Up the Other is Down; 1.4 Mythical Failures of VB Theory: More Ground is Gained by MO Theory; 1.5 Are the Failures of VB Theory Real?; 1.5.1 The O(2) Failure; 1.5.2 The C(4)H(4) Failure; 1.5.3 The C(5) H(5)(+) Failure; 1.5.4 The Failure Associated with the Photoelectron Spectroscopy of CH(4) 1.6 Valence Bond is a Legitimate Theory Alongside Molecular Orbital Theory1.7 Modern VB Theory: Valence Bond Theory is Coming of Age; 2 A Brief Tour Through Some Valence Bond Outputs and Terminology; 2.1 Valence Bond Output for the H(2) Molecule; 2.2 Valence Bond Mixing Diagrams; 2.3 Valence Bond Output for the HF Molecule; 3 Basic Valence Bond Theory; 3.1 Writing and Representing Valence Bond Wave Functions; 3.1.1 VB Wave Functions with Localized Atomic Orbitals; 3.1.2 Valence Bond Wave Functions with Semilocalized AOs; 3.1.3 Valence Bond Wave Functions with Fragment Orbitals 3.1.4 Writing Valence Bond Wave Functions Beyond the 2e/2c Case3.1.5 Pictorial Representation of Valence Bond Wave Functions by Bond Diagrams; 3.2 Overlaps between Determinants; 3.3 Valence Bond Formalism Using the Exact Hamiltonian; 3.3.1 Purely Covalent Singlet and Triplet Repulsive States; 3.3.2 Configuration Interaction Involving Ionic Terms; 3.4 Valence Bond Formalism Using an Effective Hamiltonian; 3.5 Some Simple Formulas for Elementary Interactions; 3.5.1 The Two-Electron Bond; 3.5.2 Repulsive Interactions in Valence Bond Theory; 3.5.3 Mixing of Degenerate Valence Bond Structures 3.5.4 Nonbonding Interactions in Valence Bond Theory3.6 Structural Coefficients and Weights of Valence Bond Wave Functions; 3.7 Bridges between Molecular Orbital and Valence Bond Theories; 3.7.1 Comparison of Qualitative Valence Bond and Molecular Orbital Theories; 3.7.2 The Relationship between Molecular Orbital and Valence Bond Wave Functions; 3.7.3 Localized Bond Orbitals: A Pictorial Bridge between Molecular Orbital and Valence Bond Wave Functions; Appendix; 3.A.1 Normalization Constants, Energies, Overlaps, and Matrix Elements of Valence Bond Wave Functions 3.A.1.1 Energy and Self-Overlap of an Atomic Orbital-Based Determinant3.A.1.2 Hamiltonian Matrix Elements and Overlaps between Atomic Orbital-Based Determinants; 3.A.2 Simple Guidelines for Valence Bond Mixing; Exercises; Answers; 4 Mapping Molecular Orbital-Configuration Interaction to Valence Bond Wave Functions; 4.1 Generating a Set of Valence Bond Structures; 4.2 Mapping a Molecular Orbital-Configuration Interaction Wave Function into a Valence Bond Wave Function; 4.2.1 Expansion of Molecular Orbital Determinants in Terms of Atomic Orbital Determinants 4.2.2 Projecting the Molecular Orbital-Configuration Interaction Wave Function Onto the Rumer Basis of Valence Bond Structures
Sommario/riassunto	This reference on current VB theory and applications presents a practical system that can be applied to a variety of chemical problems in a uniform manner. After explaining basic VB theory, it discusses VB applications to bonding problems, aromaticity and antiaromaticity, the dioxygen molecule, polyradicals, excited states, organic reactions, inorganic/organometallic reactions, photochemical reactions, and catalytic reactions. With a guide for performing VB calculations, exercises and answers, and numerous solved problems, this is the premier reference for practitioners and upper-level student