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Titolo	Valence bond methods : theory and applications / / Gordon A. Gallup [[electronic resource]]
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Nota di contenuto	; Part I. Theory and Two-Electron Systems: -- . Introduction -- H2 and localised orbitals -- H2 and delocalised orbitals -- Three electrons in doublet states -- Advanced methods for larger molecules -- Spatial symmetry -- Varieties of valence bond treatments -- Physics of ionic structures -- ; Part II. Examples and Interpretations: -- Selection of structures and arrangement of bases -- Four simple three-electron systems -- Second row homonuclear diatomics -- Second row heteronuclear diatomics -- Methane, ethane and hybridization -- Rings of hydrogen atoms -- Aromatic compounds -- Interaction of molecular fragments -- Appendix.
Sommario/riassunto	Valence bond theory is one of two commonly used methods in molecular quantum mechanics, the other is molecular orbital theory. This book focuses on the first of these methods, ab initio valence bond theory. The book is split into two parts. Part I gives simple examples of two-electron calculations and the necessary theory to extend these to

larger systems. Part II gives a set of case studies of related molecule sets designed to show the nature of the valence bond description of molecular structure. It also highlights the stability of this description to varying basis sets. There are references to the CRUNCH computer program for molecular structure calculations which is currently available in the public domain. The book will be of primary interest to researchers and students working on electronic theory and computation in chemistry and chemical physics.