1. Record Nr. UNINA9910140807403321 Autore Magnasco Valerio **Titolo** Models for bonding in chemistry [[electronic resource] /] / Valerio Magnasco Hoboken,: Wiley, 2010 Pubbl/distr/stampa 1-282-77312-7 **ISBN** 9786612773129 1-119-95734-6 1-119-97198-5 0-470-66975-6 Descrizione fisica 1 online resource (234 p.) Disciplina 541/.224 Soggetti Chemical bonds Molecular structure - Mathematical models Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Description based upon print version of record. Includes bibliographical references and index. Nota di bibliografia Nota di contenuto Models for Bonding in Chemistry; Contents; Preface; 1 Mathematical Foundations: 1.1 MATRICES AND SYSTEMS OF LINEAR EQUATIONS: 1.2 PROPERTIES OF EIGENVALUES AND EIGENVECTORS: 1.3 VARIATIONAL APPROXIMATIONS: 1.4 ATOMIC UNITS: 1.5 THE ELECTRON DISTRIBUTION IN MOLECULES; 1.6 EXCHANGE-OVERLAP DENSITIES AND THE CHEMICAL BOND; Part 1: Short-range Interactions; 2 The Chemical Bond; 2.1 AN ELEMENTARY MOLECULAR ORBITAL MODEL; 2.2 BOND ENERGIES AND PAULI REPULSIONS IN HOMONUCLEAR DIATOMICS: 2.2.1 The Hydrogen Molecular Ion H+2 (N = 1); 2.2.2 The Hydrogen Molecule H2(N = 2)2.2.3 The Helium Molecular Ion He+2 (N = 3)2.2.4 The Helium Molecule He2 (N = 4); 2.3 MULTIPLE BONDS; 2.3.1 s2p2 Description of the Double Bond; 2.3.2 B 2 1 B 2 2 Bent (or Banana) Description of the Double Bond: 2.3.3 Hybridization Effects: 2.3.4 Triple Bonds: 2.4 THE THREE-CENTRE DOUBLE BOND IN DIBORANE; 2.5 THE HETEROPOLAR BOND; 2.6 STEREOCHEMISTRY OF POLYATOMIC MOLECULES; 2.6.1 The

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A readable little book assisting the student in understanding, in a nonmathematical way, the essentials of the different bonds occurring in chemistry. Starting with a short, self-contained,introduction, Chapter 1 presents the essential elements of the variation approach to either total or second-order molecular energies, the system of atomic units (au) necessary to simplify all mathematical expressions, and an introductory description of the electron distribution in molecules. Using mostly 2x2 Huckel secular equations, Chapter 2, by far the largest part of the book because of the many implicat

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