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Autore	Magnasco Valerio
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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 H ₂ (N = 2) 2.2.3 The Helium Molecular Ion He ⁺ 2 (N = 3)2.2.4 The Helium Molecule He ₂ (N = 4); 2.3 MULTIPLE BONDS; 2.3.1 s ² p ² 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 Molecular Orbital Model of Directed Valency; 2.6.2 Analysis of the MO Bond Energy; 2.7 sp-HYBRIDIZATION EFFECTS IN FIRST-ROW HYDRIDES; 2.7.1 The Methane Molecule; 2.7.2 The Hydrogen Fluoride Molecule 2.7.3 The Water Molecule 2.7.4 The Ammonia Molecule; 2.8 DELOCALIZED BONDS; 2.8.1 The Ethylene Molecule; 2.8.2 The Allyl Radical; 2.8.3 The Butadiene Molecule; 2.8.4 The Cyclobutadiene Molecule; 2.8.5 The Benzene Molecule; 2.9 APPENDICES; 2.9.1 The Second Derivative of the Hückel Energy; 2.9.2 The Set of Three Coulson's Orthogonal Hybrids; 2.9.3 Calculation of Coefficients of Real MOs for Benzene; 3 An Introduction to Bonding in Solids; 3.1 THE LINEAR POLYENE CHAIN; 3.1.1 Butadiene $N = 4$; 3.2 THE CLOSED POLYENE CHAIN; 3.2.1 Benzene $N = 6$; 3.3 A MODEL FOR THE ONE-DIMENSIONAL CRYSTAL 3.4 ELECTRONIC BANDS IN CRYSTALS 3.5 INSULATORS, CONDUCTORS, SEMICONDUCTORS AND SUPERCONDUCTORS; 3.6 APPENDIX: THE TRIGONOMETRIC IDENTITY; Part 2: Long-Range Interactions; 4 The van der Waals Bond; 4.1 INTRODUCTION; 4.2 ELEMENTS OF RAYLEIGH-SCHRODINGER (RS) PERTURBATION THEORY; 4.3 MOLECULAR INTERACTIONS; 4.3.1 Non-expanded Energy Corrections up to Second Order; 4.3.2 Expanded Energy Corrections up to Second Order; 4.4 THE TWO-STATE MODEL OF LONG-RANGE INTERACTIONS; 4.5 THE van der WAALS INTERACTIONS; 4.5.1 Atom-Atom Dispersion; 4.5.2 Atom-Linear Molecule Dispersion 4.5.3 Atom-Linear Dipolar Molecule 4.6 THE C_6 DISPERSION COEFFICIENT FOR THE H-H INTERACTION; 4.7 THE van der WAALS BOND; 4.8 THE KEESOM INTERACTION; 5 The Hydrogen Bond; 5.1 A MOLECULAR ORBITAL MODEL OF THE HYDROGEN BOND; 5.2 ELECTROSTATIC INTERACTIONS AND THE HYDROGEN BOND; 5.2.1 The Hydrogen Fluoride Dimer (HF)₂; 5.2.2 The Water Dimer (H₂O)₂; 5.3 THE ELECTROSTATIC MODEL OF THE HYDROGEN BOND; 5.4 THE Rg-HF HETERODIMERS; References; Author Index; Subject Index

Sommario/riassunto

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