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Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Contents; PART I: FUNDAMENTALS; 1 The molecule: structure, size and shape; 1.1 Atoms and bonds; 1.2 Classification concepts in many particle systems; 1.3 Must a molecule have a size?; 1.4 Must a molecule have a shape?; 1.5 Historical portraits: a chemistry course in the early 1960's; 2 Molecular vibrations and molecular force fields; 2.1 Vibrational modes and force constants; 2.2 Molecular mechanics; 2.3 Evolution of molecular force fields; 2.4 Appendix: an example of coordinate transformation; 2.5 Historical portraits: Got a force constant?; 3 Quantum chemistry 3.1 Some fundamentals of quantum mechanics 3.2 The hydrogen atom and atomic orbitals; 3.3 Spin; 3.4 Many-electron systems; 3.5 Molecular orbitals: The Fock and Roothaan equations; 3.6 Approximate quantum chemical methods: NDO and EHT; 3.7 Evolution of quantum chemical calculations: Beyond Hartree-Fock; 3.8 Dimerization energies

and basis set superposition error; 3.9 Historical portraits: early experiences in quantum chemistry; 4 The physical nature and the computer simulation of the intermolecular potential; 4.1 Experimental facts and conceptual framework
4.2 The representation of the molecular charge distribution and of the electric potential 4.3 Coulombic potential energy; 4.4 Polarization (electrostatic induction) energy; 4.5 Dispersion energy; 4.6 Pauli (exchange) repulsion energy; 4.7 Total energies versus partitioned energies; 4.8 Intermolecular hydrogen bonding; 4.9 Simulation methods; 4.10 Ad hoc or transferable? Force field fitting from ab initio calculations; 5 Crystal symmetry and X-ray diffraction; 5.1 A structural view of crystal symmetry: bottom-up crystallography; 5.2 Space group symmetry and its mathematical representation
5.3 von Laue's idea, 1912 5.4 The structure factor; 5.5 Miller indices and Bragg's law; 5.6 The electron density in a crystal; 5.7 The atomic prejudice; 5.8 Structure and X-ray diffraction: Some examples; 5.9 Historical portraits: Training of a crystallographer in the 1960's; 6 Periodic systems: Crystal orbitals and lattice dynamics; 6.1 The mathematical description of crystal periodicity; 6.2 The electronic structure of solids; 6.3 Lattice dynamics and lattice vibrations; 7 Molecular structure and macroscopic properties: Calorimetry and thermodynamics; 7.1 Molecules and macroscopic bodies
7.2 Energy 7.3 Heat capacity; 7.4 Entropy; 7.5 Free energy and chemical equilibrium; 7.6 Thermodynamic measurements; 7.7 Derivatives; 8 Correlation studies in organic solids; 8.1 The Cambridge Structural Database (CSD) of organic crystals; 8.2 Structure correlation; 8.3 Retrieval of molecular and crystal structures from the CSD; 8.4 The SubHeat database; 8.5 The geometrical categorization of intermolecular bonding; 8.6 Space analysis of molecular packing modes; 8.7 The calculation of intermolecular energies in crystals; 8.8 General-purpose force fields for organic crystals
8.9 Accuracy and reproducibility

Sommario/riassunto

The book is divided in two parts, to supply first the basic elements of the language, with short but complete explanations of terms, methods and theories; and then to describe the present status of studies on the processes by which organic molecules aggregate to form observable bodies and to determine their physical and chemical properties. - ;This book is divided in two parts. Part I provides a brief but accurate summary of all the basic ideas, theories, methods, and conspicuous results of structure analysis and molecular modelling of the condensed phases of organic compounds: quantum chemist