

1. Record Nr.	UNINA9910145283203321
Autore	Bakhmutov Vladimir I
Titolo	Dihydrogen bonds [[electronic resource]] : principles, experiments, and applications / / Vladimir I. Bakhmutov
Pubbl/distr/stampa	Hoboken, N.J., : Wiley-Interscience, c2008
ISBN	1-281-23728-0 9786611237288 0-470-22675-7 0-470-22674-9
Descrizione fisica	1 online resource (257 p.)
Disciplina	541.226
Soggetti	Dihydrogen bonding
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	DIHYDROGEN BONDS; CONTENTS; Preface; 1 Introduction: Weak Noncovalent Interactions; References; 2 Brief Summary of Hydrogen-Bonded Systems: Definitions and General View; 2.1 Conventional Hydrogen Bonds: Theoretical and Experimental Criteria of Hydrogen Bond Formation; 2.1.1 Energy and Geometry of Conventional Hydrogen Bonds; 2.1.2 Cooperative and Anticooperative Energy Effects in Systems with Classical Hydrogen Bonds; 2.1.3 Dynamics of Classical Hydrogen Bonds; 2.2 Nonconventional Hydrogen Bonds as a Part of Hydrogen-Bonded Systems: Definition and Classification 2.3 Difference Between Hydrogen and Chemical Bonds 2.4 Concluding Remarks; References; 3 Concept of Dihydrogen Bonding; 3.1 General View: From an H(2) Molecule to a Dihydrogen Bond via a Dihydrogen Ligand; 3.2 The Nature of Dihydrogen Bonding: The Topology of Electron Density and Contributions to Total Bonding Energy; 3.3. Scalar Spin-Spin Coupling Through Dihydrogen Bonds as Evidence of Their Partly Covalent Character; 3.4 Field Effects on Dihydrogen Bonding; 3.5 Pressure Effects on Dihydrogen Bonding; 3.6 Difference Between Hydrogen and Dihydrogen Bonds; 3.7 Concluding Remarks; References 4 How to Find a Dihydrogen Bond: Experimental Criteria of Dihydrogen Bond Formation 4.1 Dihydrogen-Bonded Complexes in the Solid State: X-Ray and Neutron Diffraction Evidence; 4.1.1 Topology of Electron

Density in Dihydrogen-Bonded Systems from Diffraction Data; 4.2 Gas-Phase Experiments with Dihydrogen-Bonded Complexes; 4.3 Experiments with Dihydrogen-Bonded Complexes in Solutions; 4.3.1 IR Spectral Criteria for the Formation of Dihydrogen-Bonded Complexes in Solutions; 4.3.2 How to Determine the Stoichiometry of Dihydrogen-Bonded Complexes in Solution by IR Spectroscopy 4.3.3 Energy Parameters of Dihydrogen-Bonded Complexes from IR Spectra in Solution 4.3.4 (1)H Nuclear Magnetic Resonance Evidence for Dihydrogen Bonding in Solution; 4.3.5 Energy Parameters of Dihydrogen Bonds in Solution from (1)H NMR; 4.4 Concluding Remarks; References; 5 Intramolecular Dihydrogen Bonds: Theory and Experiment; 5.1 Weak Intramolecular Bonding: C-H· · ·H-C in Systems with Slightly Polarized Bonds CH; 5.2 Intramolecular Dihydrogen Bonds in Solid Amino Acids: C-H Bonds as Weak Proton Acceptors; 5.3 Intramolecular Dihydrogen Bonds: C-H· · ·H-B 5.4 Intramolecular Bonds: N-H· · ·H-B and O-H· · ·H-B 5.5 Intramolecular Dihydrogen Bonds in Metal Hydride Complexes; 5.5.1 Intramolecular Dihydrogen Bonds in Metal Hydride Clusters; 5.6 Connection Between Intramolecular Dihydrogen Bonding and Dehydrogenation Reactions; 5.7 Concluding Remarks; References; 6 Intermolecular Dihydrogen-Bonded Complexes: From Groups 1A-4A to Xenon Dihydrogen-Bonded Complexes; 6.1 Group 1A: Dihydrogen Bonds X-H· · ·H-Li and X-H· · ·H-Na (X = F, Cl, NH(3), CN, NC, HO, HS, CICC, FCC, HCC) 6.2 Group 2A: Dihydrogen Bonds X-H· · ·H-Mg and X-H· · ·H-Be (X = F, Cl, Br, NH(3), NNN, CN, NC, CICC, FCC, HCC, CH(3)CC, F(2)Be, FKr, FAr)

Sommario/riassunto

This definitive reference consolidates current knowledge on dihydrogen bonding, emphasizing its role in organizing interactions in different chemical reactions and molecular aggregations. After an overview, it analyzes the differences between dihydrogen bonds, classical hydrogen bonds, and covalent bonds. It describes dihydrogen bonds as intermediates in intramolecular and intermolecular proton transfer reactions. It describes dihydrogen bonding in the solid-state, the gas phase, and in solution. This is the premier reference for physical chemists, biochemists, biophysicists, and chemical engi