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G5S9SS - MAXWELL ODONNELL

Hydrogen bond (H-bond) effects are known: it makes sea water liquid, joins cellulose microfibrils in trees, shapes DNA into genes and polypeptide chains into wool, hair, muscles or enzymes. Its true nature is less known and we may still wonder why O-H…O bond energies range from less

than 1 to more than 30 kcal/mol without apparent reason. This H-bond puzzle is re-examined here from its very beginning and presented as an inclusive compilation of experimental H-bond energies and geometries. New concepts emerge from this analysis: new classes of systematically strong H-bonds (CAHBs and RAHBs: charge- and resonance-assisted H-bonds); full H-bond classification in six classes (the six chemical leitmotifs); and assessment of the covalent nature of strong H-bonds. This leads to three distinct but inter-consistent models able to rationalize the H-bond and predict its strength, based on classical VB theory, matching of donor-acceptor acid-base parameters (PA or pKa), or shape of the H-bond proton-transfer pathway. Applications survey a number of systems where strong H-bonds play an important functional role, namely drug-receptor binding, enzymatic catalysis, ion-transport through cell membranes, crystal design and molecular mechanisms of functional materials.

This book uses examples from experimental studies to illustrate theoretical investigations, allowing greater understanding of hydrogen bonding phenomena. The most important topics in recent studies are covered. This volume is an invaluable resource that will be of particular interest to physical and theoretical chemists, spectroscopists, crystallographers and those involved with chemical physics.

Hydrogen in Steel: Effect of Hydrogen on Iron and Steel During Production, Fabrication, and Use focuses on the effect of hydrogen on iron and steel during production, fabrication, and use. Topics covered range from the solubility of hydrogen in iron and ferrous alloys to the diffusion and permeation of hydrogen through iron and steel. Electrochemical problems related to the ability of iron to absorb hydrogen from aqueous solutions are also considered. Comprised of 19 chapters, this book begins with a detailed treatment of the nature and properties of metal-hydrogen systems, paying particular attention to the behavior of hydrogen in the bulk of the metal phase and the mechanism of reactions between metals and hydrogen or hydrogen-producing compounds. The reader is then introduced to the solubility of hydrogen in iron and ferrous alloys as well as the nature of the final product of the hydrogen-iron interaction. Subsequent chapters deal with dimensional changes and stresses produced in steel by cathodically evolved hydrogen; the effects of hydrogen on the physical, mechanical, and chemical properties of iron and steel; influence of welding on hydrogen; and sulfide corrosion cracking of steel. The effects of pickling on steel are also examined, along with the blistering and embrittlement caused by hydrogen on the base metal during electroplating. This book will be of value to students and practitioners in the field of physical chemistry.

Unusually clear, accessible introduction to contemporary theories of solid-state physics. Nonmathematical treatment of heat, atomic motion, electrons in solids, many other topics. "Excellent." -- "Choice." 1965 edition.

Materials Science Forum Vol. 31

One of the first books dedicated to the emerging field of neutron protein crystallography (NPC). It covers all of the practical aspects of NPC and demonstrates how NPC can explore protein features such as hydrogen bonds, protonation and deprotonation of amino acid residues, and hydra-

tion structures.

The importance of hydrogen bond interactions in many chemical and biological processes such as aqueous solvation and reaction, atmospheric aerosol formation and reactivity, and enzyme functionality has fueled an increasing interest in the field of hydrogen bonded liquids. Clusters of hydrogen bonded systems serve as prototypes in obtaining a molecular level understanding of their stability and chemical reactivity via the exploration of their structural and dynamical properties. Since they probe the fundamental interactions at the molecular level, they furthermore offer the advantage of serving as guidelines/benchmarks in the development of comprehensive models used to simulate the measured macroscopic properties of condensed phase environments. To this end, theory and experiment enter as equal partners in the effort to provide a broader picture of the nature of the hydrogen bond in clusters with the ultimate goal of modeling processes in condensed phase environments of these systems. Theory is needed in order to provide a vehicle for the interpertation of the experimental measurements and, in turn, experimental validation of the theoretical propositions strengthens their credibility.

A look at the make up of matter, the states of matter and the physical and chemical properties of matter.

The author illustrates why the rather weak hydrogen bond is so essential for our everyday life in a lively and entertaining way. The chemical and physical fundamentals are explained with examples ranging from the nature of water over the secret of DNA to adhesives and modern detergents. The interdisciplinary science is easy to understand and hence a great introduction for chemists, biologists and physicists.

This book gives an extensive description of the state-of-the-art in research on excited-state hydrogen bonding and hydrogen transfer in recent years. Initial chapters present both the experimental and theoretical investigations on the excited-state hydrogen bonding structures and dynamics of many organic and biological chromophores. Following this, several chapters describe the influences of the excited-state hydrogen bonding on various photophysical processes and photochemical reactions, for example: hydrogen bonding effects on fluorescence emission behaviors and photoisomerization; the role of hydrogen bonding in photosynthetic water splitting; photoinduced electron transfer and solvation dynamics in room temperature ionic liquids; and hydrogen bonding barrier crossing dynamics at bio-mimicking surfaces. Finally, the book examines experimental and theoretical studies on the nature and control of excited-state hydrogen transfer in various systems. Hydrogen Bonding and Transfer in the Excited State is an essential overview of this increasingly important field of study, surveying the entire field over 2 volumes, 40 chapters and 1200 pages. It will find a place on the bookshelves of researchers in photochemistry, photobiology, photophysics, physical chemistry and chemical physics.

As one of the typical intermolecular interactions, hydrogen-bonding plays a significant role in molecular structure and function. When the hydrogen bond research system is connected with the photon, the hydrogen-bonding effect turns to an excited-state one influencing photochemistry, photobiology, and photophysics. Thus, the

hydrogen bond in an excited state is a key topic for understanding the excited-state properties, especially for optoelectronic or luminescent materials.The approaches presented in this book include quantum chemical calculation, molecular dynamics simulation and ultrafast spectroscopy, which are strong tools to investigate the hydrogen bond. Unlike other existing titles, this book combines theoretical calculations and experiments to explore the nature of excited-state hydrogen bonds. By using these methods, more details and faster processes involved in excited-state dynamics of hydrogen bond are explored.This highly interdisciplinary book provides an overview of leading hydrogen bond research. It is essential reading for faculties and students in researching photochemistry, photobiology and photophysics, as well as novel optoelectronic materials, fluorescence probes and photocatalysts. It will also guide research beginners to getting a quick start within this field.

There continues to be widespread interest in the applications of hydrogen as a clean fuel and its potential for local electricity production and use in transport. Recent years have seen a variety of breakthroughs in our understanding of the nature, structure, and biosynthesis of hydrogenases. This book is a timely description of these developments,

This book defines, for the first time, the rules for predicting H-bond energies and geometries from the properties of the interacting molecules. This new knowledge is used to investigate the molecular mechanisms in systems relevant to chemistry, biochemistry, pharmacology, crystallography, and material sciences.