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Hydrogen Bonding

MARQUIS JORDON

Hydrogen Bonds John Wiley & Sons
Hydrogen bonds range from the very strong, comparable with covalent bonds, to the very weak, comparable with van der Waals forces. Most hydrogen bonds are weak attractions with a binding strength about one-tenth of that of a normal covalent bond. Nevertheless, they are very important. Without them, all wooden structures would collapse, cement would crumble, oceans would vaporize, and all living things would disintegrate into inanimate matter. An easy-to-read supplement to the often brief descriptions of hydrogen bonding found in most undergraduate chemistry and molecular biology textbooks, An Introduction to Hydrogen Bonding describes and discusses the current ideas concerning hydrogen bonding, ranging from the very strong to the very weak, with introductions to the experimental and theoretical methods involved. Ideal for courses in chemistry and biochemistry, it will also be useful for structural biology and crystallography courses. For students and researchers interested in supramolecular chemistry, biological structure and recognition, and other sophisticated concepts and methodologies, it provides a careful selection of key references from the vast hydrogen bonding literature.
Visualization of Hydrogen-Bond Dynamics World Scientific
Hydrogen bonds represent type of molecular interaction that determines the structure and function of a large variety of molecular systems. The elementary dynamics of hydrogen bonds and related proton transfer reactions, both occurring in the ultra fast time domain between 10-14 and 10-11s, form a research topic of high current interest. In this book addressing scientists and graduate students in physics, chemistry and biology, the ultra fast dynamics of hydrogen bonds and proton transfer in the condensed phase are reviewed by leading scientists, documenting the state of the art in this exciting field from the viewpoint of theory and experiment. The nonequilibrium behavior of hydrogen-bonded liquids and intramolecular hydrogen bonds as well as photo induced hydrogen and proton transfer are covered in 7 chapters, making reference to the most recent literature.
The Nature of the Hydrogen Bond World Scientific
This first comprehensive overview of the rapidly growing field emphasizes the use of hydrogen bonding as a tool for organic synthesis, especially catalysis. As such, it covers such topics as enzyme chemistry, organocatalysis and total synthesis, all unified by the unique advantages of hydrogen bonding in the construction of complex molecules from simple precursors. Providing everything you need to know, this is a definite must for every synthetic chemist in academia and industry.
Analysis of Hydrogen Bonds in Crystals Springer Science & Business Media
The book illustrates the fascinating world of the different forms of water - from ice and snow to liquid water. The water molecule, H2O, is the second most common molecule in the Universe (behind hydrogen, H2) and ice is the most abundant solid material. Snow and

ice appear in a countless large number of different shapes and with properties which can be quite different. Detailed knowledge of the properties of snow is of great importance for the Sami people involved in reindeer herding and several hundred names are used to characterize the different types. The properties of ice and liquid water are very special and unique in several respects. In contrast to most other substances, the density of ice is lower than that of liquid water, which has many very important consequences in our daily life. Water plays a unique role in chemistry and although tremendous research has been spent on this seemingly simple substance, there are still many unsolved questions about the structure of liquid water. The special properties of water are due to hydrogen bonding between the H2O molecules, and this book may be seen as a tribute to the hydrogen bond. The general properties of the hydrogen bond are treated in three separate papers. The hydrogen bond is of fundamental importance in biological systems since all living matter has evolved from and exists in an aqueous environment and hydrogen bonds are involved in most biological processes. There is a hundred times more water molecules in our bodies than the sum of all the other molecules put together. -- Provided by publisher.

Non-Covalent Catalysis and Hydrogen Bonding Springer Science & Business Media

This monograph describes the behavior of molecules confined to small spaces. The small spaces are created by the self-assembly of modules into hollow capsular structures through hydrogen bonding; capsules assembled by metal/ligand binding or other forces are not included. Topics discussed include how assembly of capsules occurs, how molecules get in and out of the capsules, new spatial arrangements (stereochemistry) created in the capsules, and the altered shapes, interactions and reactivities of molecules held inside the small spaces. The descriptions emphasize molecular recognition phenomena and the perspective is that of physical organic chemistry. The book is the first monograph to treat reversible molecular encapsulation. More than 20 university and institute groups worldwide engage in this research, which represents the leading edge of activity in molecular recognition and the physical organic chemistry of confined molecules. Contents:Spherical and Similar CapsulesCalixarene CapsulesThe Cylindrical CapsuleHexameric Capsules from Resorcinarenes and PyrogallolarenesStereochemistry of Confined MoleculesChiral CapsulesExpanded and Contracted CapsulesReactions Inside Capsules Readership: Graduate students and researchers in physical organic chemistry, nanotechnology and nanoscience and materials science. Keywords:Capsules;Encapsulation;Recognition;Reactivity;Stereochemistry;Resorcinarenes;Calixarenes;Dynamics;Thermodynamics Key Features:The last monograph to deal with molecules inside molecules was published in 1994. Hydrogen bonded capsules have been invented since that time and this monograph summarizes the results of more than 100 publications in this fieldMolecules in small spaces behave differently than those that are free in solution; this monograph reveals these new behaviors and draws parallels to the related behavior of small molecules confined in enzymes and biological

receptorsThe monograph provides recipes for construction of molecular devices at the sub-nano scale. The principles of self-assembly are involved and offer applications in nanoscience using an approach "from the bottom up" *Hydrogen Bonding and Transfer in the Excited State* Garland Science
Hydrogen Bonding covers the papers presented at the Symposium on Hydrogen Bonding, held at Ljubljana on July 29 to August 3, 1957. The book focuses on the developments, processes, approaches, methodologies, and reactions involved in hydrogen bonding. The selection first offers information on the structure of water; function of hydrogen bond in solids and liquids; and study of hydrogen bonds by neutron diffraction. The text then takes a look at x-ray and neutron studies of hydrogen bonding; x-ray studies of ammonium bifluoride, potassium hydrogen maleate, theophylline, and caffeine; and isotope effect in relation to bond length in hydrogen bonds in crystals. The publication ponders on proton magnetic resonance measurements of hydrogen bonding; interpretation of nuclear magnetic resonance shifts in hydrogen bonding; nuclear resonance investigation of hydrogen bonding; and infrared spectroscopy and hydrogen bonding — band-widths and frequency shifts. The book then examines the tunneling of protons as a cause of the splitting of hydroxyl stretching bands; infrared spectroscopic study of H-bonding and of metal-element bonding; and effect of hydrogen bond formation on the electronic spectra of phenolic substances. The selection is a vital source of information for readers interested in hydrogen bonding.
Hydrogen-bonded Capsules Elsevier
The almost universal presence of water in our everyday lives and the very `common' nature of its presence and properties possibly deflects attention from the fact that it has a number of very unusual characteristics which, furthermore, are found to be extremely sensitive to physical parameters, chemical environment and other influences. Hydrogen-bonding effects, too, are not restricted to water, so it is necessary to investigate other systems as well, in order to understand the characteristics in a wider context. Hydrogen Bond Networks reflects the diversity and relevance of water in subjects ranging from the fundamentals of condensed matter physics, through aspects of chemical reactivity to structure and function in biological systems.
Supramolecular Assembly Via Hydrogen Bonds I Oxford University Press on Demand
This book is intended as an easy to read supplement to the often brief descriptions of hydrogen bonding found in most undergraduate chemistry and molecular biology textbooks. It describes and discusses current ideas concerning hydrogen bonds ranging from the very strong to the very weak, with introductions to the experimental and theoretical methods involved.
Dissecting the Physical and Energetic Properties of Active Site Hydrogen Bonds in Ketosteroid Isomerase Oxford University Press
Hydrogen bonded systems play an important role in all aspects of science but particularly chemistry and biology. Notably, the helical structure of DNA is heavily reliant on the hydrogens bonds between the DNA base pairs. Although the area of hydrogen bonding is one that is well established, our understanding has continued to develop as the power

of both computational and experimental techniques has improved. Understanding Hydrogen Bonds presents an up-to-date overview of our theoretical and experimental understanding of the hydrogen bond. Well-established and novel approaches are discussed, including quantum theory of ‘atoms in molecules’ (QTAIM); the electron localization function (ELF) method and Car–Parinnello molecular dynamics; the natural bond orbital (NBO) approach; and X-ray and neutron diffraction and spectroscopy. The mechanism of hydrogen bond formation is described and comparisons are made between hydrogen bonds and other types of interaction. The author also takes a look at new types of interaction that may be classified as hydrogen bonds with a focus on those with multicentre proton acceptors or with multicentre proton donors. Understanding Hydrogen Bonds is a valuable reference for experimentalists and theoreticians interested in updating their understanding of the types of hydrogen bonds, their role in chemistry and biology, and how they can be studied.
Cell Biology by the Numbers John Wiley & Sons
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.
An Introduction to Hydrogen Bonding GRIN Verlag
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.
An Introduction to Hydrogen Bonding Springer Science & Business Media
The book presents the fantastic world of water in all its different forms, from liquid to ice and snow. This book is amply illustrated with a large number of beautiful pictures with. Water plays a unique role in chemistry. The special properties of water are due to hydrogen bonding between the H2O molecules. The hydrogen bond is of fundamental importance in biological systems since all living matter has evolved from and exists in an aqueous environment, and

hydrogen bonds are involved in most biological processes. There is a hundred times more water molecules in our bodies than the sum of all the other molecules put together. The unique properties of water are of great importance in our daily life. The origin of these special properties is often not recognized. Even among chemists and physicists, the fundamental facts are not always known. In spite of very active research, there are still many questions to be answered about the structure of liquid water, for instance. The book differs from most books on water as it covers basic facts about structure and properties as well as the influence of these properties in our daily life. Why does ice float on water? Why is the maximum density of water at 4°C? The beauty of snow crystals is amply illustrated, and many of the pictures are unique. Contents: Early Snow Crystal ObservationsArtificially Grown Snow CrystalsTwins, Snowflakes and HailFormation of RainPictures of Snow and Ice Crystals in NatureSnow for Pleasure and ArtThe Ice Surface and Formation of Ice SpikesIce as Aircraft Carrier and Project HabakkukStructure of Water and IcePhysical Properties and Significance in NatureWater, a Solvent with Many Interesting PropertiesWhy is Water Blue?Electron Microscopic Studies of Snow CrystalsIce in Lakes and GlaciersHydrates of Methane, Carbon Dioxide and ChlorineEffects Connected with the Release of MethanePolyhedra Formed by Water, Carbon and HydrocarbonsThe Platonic SolidsMysteries of WaterEscher's Waterfall and the Impossible TriangleMemory of WaterJacques BenvenisteHomeopathyMasaru EmotoCan Warm Water Freeze Faster than Cold Water?Mpemba Effects in Our Daily LifeHot-Water Pipes Break on Freezing While Cold Ones Do Not!The Hydrogen BondThe Role of the Lone-Pair Electrons on the Acceptor AtomThe Hydrated ProtonWater in Biological SystemsWater Transport in TreesTransformations of Our Earth by Water and IceIce AgesGiant's Kettles, PotholesThe Story of Döda Fallet (The 'Dead Fall')The Rain BowThe Physical Origin of the RainbowTeoderick's Rainbow ExperimentPrimary and Secondary RainbowsThe Water Molecule is Unique Readership: Interested lay readers. Keywords: Water;Hydrogen Bond;Ice;Snow;Gas Hydrates;Mysteries of Water;Mpemba Effect;RainbowReview:0

Intermolecular Forces Oxford University Press

Hydrogen bonds are a ubiquitous feature of enzyme active sites, stabilizing charge rearrangements on substrate groups over the course of a reaction. Although their importance is clear from traditional site-directed mutagenesis, understanding the origin of their catalytic contribution relative to hydrogen bonds made in aqueous solution remains challenging, in part because traditional mutagenesis ablates hydrogen bonding groups or replaces them with hydrophobic side chains, rendering comparisons between wild type and mutant enzymes complex. Additional complexity arises from the extraordinary sensitivity of hydrogen bond energetics to the surrounding environment. In this thesis, I describe how I substituted tyrosine (Tyr) with fluorotyrosines (F-Tyr's) in the ketosteroid isomerase (KSI) oxyanion hole to systematically vary the proton affinity of an active site hydrogen bond donor while minimizing steric or structural effects and assessed the

physical and energetic consequences of this perturbation to provide powerful experimental tests of the behavior of intact hydrogen bonds within an enzyme active site. I observed that a 40-fold increase in F-Tyr acidity caused no significant change in activity for reactions with three different substrates. UV/Vis absorbance and proton NMR spectra of F-Tyr-substituted KSI variants with bound transition state analogs showed that the proton affinity of the tyrosyl group and the physical properties of the Tyr hydrogen bond vary with fluoro-substitution, as expected. Additionally, the change in NMR chemical shift observed was the same as that previously observed in other solvents, providing strong evidence for the effects of fluoro-substitution not being muted by the active site environment. I found that the physical effects of F-Tyr substitution were propagated to Asp103, the other oxyanion hole residue, such that as the Tyr hydrogen bond shortens, the Asp103 hydrogen bond lengthens. This physical coupling could have masked an intrinsic steep energetic sensitivity of the Tyr hydrogen bond to charge accumulation, relative to aqueous solution, resulting in the shallow dependence of catalytic rate on F-Tyr acidity that was observed. To test this alternative model, I determined the dependence of enzymatic activity on F-Tyr acidity with Asp103 mutated to Asn or Gly, and observed the same shallow dependence as before. The observed shallow slopes provide strong evidence that the sensitivity of hydrogen bond energetics to charge accumulation within the KSI active site is not substantially greater than the low sensitivity in aqueous solution and suggest that the KSI oxyanion hole does not provide catalysis by forming an energetically exceptional "short, strong" hydrogen bond. These results are consistent with the modest but important overall catalytic contribution of the oxyanion hole residues of ~1000-fold relative to a 'pond mutant' in which these and surrounding residues are removed and are consistent with an important role of positioning of these residues by the enzyme scaffold and surrounding side chains. I close with laying out the key challenges that lie ahead in quantitatively understanding the origin of the enormous rate enhancements that enzymes provide.

Hydrogen Bonding - New Insights World Scientific

Hydrogen Bonding - New InsightsSpringer Science & Business Media

Hydrogen Bonding in Biological Structures Springer Science & Business Media

Hydrogen bonds are weak attractions, with a binding strength less than one-tenth that of a normal covalent bond. However, hydrogen bonds are of extraordinary importance; without them all wooden structures would collapse, cement would crumble, oceans would vaporize, and all living things would disintegrate into random dispersions of inert matter. Hydrogen Bonding in Biological Structures is informative and eminently usable. It is, in a sense, a Rosetta stone that unlocks a wealth of information from the language of crystallography and makes it accessible to all scientists. (From a book review of Kenneth M. Harmon, Science 1992)

Hydrogen Bonds World Scientific

Because of the importance of the hydrogen bond, there have been scores of insights gained about its fundamental nature by quantum chemical computations over the years. Such

methods can probe subtle characteristics of the electronic structure and examine regions of the potential energy surface that are simply not accessible by experimental means. The maturation of the techniques, codes, and computer hardware have permitted calculations of unprecedented reliability and rivaling the accuracy of experimental data. This book strives first toward an appreciation of the power of quantum chemistry to analyze the deepest roots of the hydrogen bond phenomenon. It offers a systematic and understandable account of decades of such calculations, focusing on the most important findings. This book provides readers with the tools to understand the original literature, and to perhaps carry out some calculations of their very own on systems of interest.
Wonders Of Water: The Hydrogen Bond In Action Oxford University Press, USA
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.
Hydrogen Bond Research John Wiley & Sons
Comprehensive spectroscopic view of the state-of the-art in theoretical and experimental hydrogen bonding research Spectroscopy and Computation of Hydrogen-Bonded Systems includes diverse research efforts spanning the frontiers of hydrogen bonding as revealed through state-of-the-art spectroscopic and computational methods, covering a broad range of experimental and theoretical methodologies used to investigate and understand hydrogen bonding. The work explores the key quantitative relationships between fundamental vibrational frequencies and hydrogen-bond length/strength and provides an extensive reference for the advancement of scientific knowledge on hydrogen-bonded systems. Theoretical models of vibrational landscapes in hydrogen-bonded systems, as well as kindred studies designed to interpret intricate spectral features in gaseous complexes, liquids, crystals, ices, polymers, and nanocomposites, serve to elucidate the provenance of spectroscopic findings. Results of experimental and theoretical studies on multidimensional proton transfer are also presented. Edited by two highly qualified researchers in the field, sample

topics covered in Spectroscopy and Computation of Hydrogen-Bonded Systems include: Quantum-mechanical treatments of tunneling-mediated pathways in enzyme catalysis and molecular-dynamics simulations of structure and dynamics in hydrogen-bonded systems Mechanisms of multiple proton-transfer pathways in hydrogen-bonded clusters and modern spectroscopic tools with synergistic quantum-chemical analyses Mechanistic investigations of deuterium kinetic isotope effects, ab initio path integral methods, and molecular-dynamics simulations Key relationships that exist between fundamental vibrational frequencies and hydrogen-bond length/strength Analogous spectroscopic and semi-empirical computational techniques examining larger hydrogen-bonded systems Reflecting the polymorphic nature of hydrogen bonding and bringing together the latest experimental and computational work in the field, Spectroscopy and Computation of Hydrogen-Bonded Systems is an essential resource for chemists and other scientists involved in projects or research that intersects with the topics covered within.

Hydrogen Bonding in Polymeric Materials Hydrogen Bonding - New Insights

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-bonding Research In Photochemistry, Photobiology, And Optoelectronic Materials Wiley Research Theoretical Che

Summarizing our current knowledge of the topic, this book describes the roles and effects of hydrogen bonding in polymer materials by reviewing the latest developments over recent years. To this end, it discusses all relevant aspects from the fundamentals, via characterization, to properties and applications in various polymeric materials, including polymer blends, block copolymers, mesoporous materials, biomacromolecules and nanocomposites. Invaluable reading for scientists in polymers and materials as well as those working in macromolecular chemistry.

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