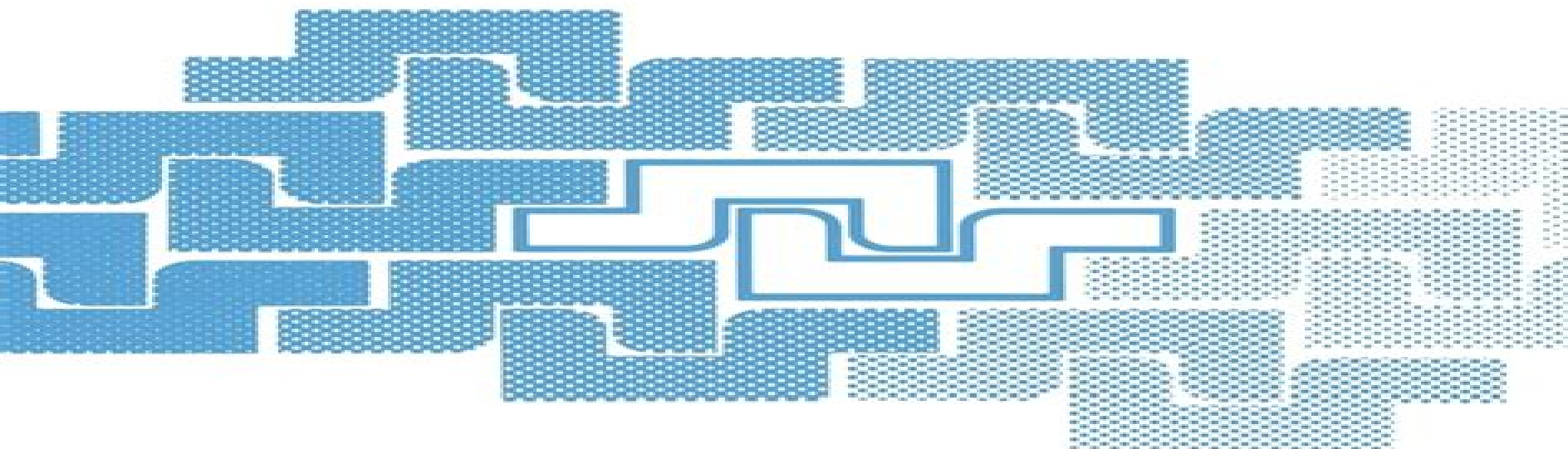




Proton Transfer in Hydrogen-Bonded Systems

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Proton Transfer In Hydrogen Bonded Systems

Simona Marincean



Proton Transfer In Hydrogen Bonded Systems:

Proton Transfer in Hydrogen-Bonded Systems T. Bountis, 2012-12-06 Charge transport through the transfer of protons between molecules has long been recognized as a fundamental process which plays an important role in many chemical reactions. In particular, proton transfer through hydrogen bonds has been identified as the main mechanism via which many biological functions are performed and many properties of such basic substances as proteins and ice can be understood. In this volume, several of these important aspects of the H bond are represented. As the division in different sections already indicates, present-day research in proton transfer in biochemistry, biology, and the physics of water and ice remains highly active and very exciting. Nearly a decade ago, a novel approach to the study of collective proton motion in H-bonded systems was proposed, in which this phenomenon was explained by the propagation of certain coherent structures called solitons. In the years that followed, the approach of soliton dynamics was further extended and developed by many researchers around the world into a legitimate and useful method for the analysis of proton transfer in H-bonded systems. Dr. Stephanos Pnevmatikos, the original Director of this ARW, was one of the pioneers in the application of soliton ideas to the study of charge transport through H bonds. Having used similar concepts himself in his research on 2D lattices, he was convinced energy transfer through molecular chains and that solitons can play an important role in enhancing our understanding of protonic conductivity.

Proton Transfer in Hydrogen-Bonded Systems T. Bountis, 1992-08-01 **Proton Transfer in Hydrogen Bonded Systems and Its Applications** Pang Xiao feng, 2013 This book presents a complete description and review of novel properties and mechanisms of form of hydrogen-bonded structure and proton transfer as well as their extensive applications in physical and biological systems. In these investigations, the properties of hydrogen bond and hydrogen-bonded system, the theory and properties of proton transfer in hydrogen-bonded systems, and its experimental evidences in ice crystal, the behaviours of hydrogen-bonded structure and proton transfer in water and gramicidin A, as well as influences of externally applied field on them, the features of hydrogen-bonded structure and soliton theory of proton transfer in DNA, and its relationship with biological functions, the biological function and molecular structure of rhodopsin and bathorhodopsin, as well as their characters of proton transfer and proton pump, are described concretely and in detail. These contents are presented and stated in five chapters respectively.

Spectroscopy and Computation of Hydrogen-Bonded Systems Marek J. Wójcik, Yukihiro Ozaki, 2022-12-27 Spectroscopy and Computation of Hydrogen Bonded Systems 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 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

Ultrafast Hydrogen Bonding Dynamics and Proton Transfer Processes in the Condensed Phase Thomas Elsaesser, H.J. Becker, 2013-03-14 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

Proton Transfer Reactions in Dihydrogen Bonded Systems Simona Marincean, 2003

Quantum Mechanics in Nonlinear Systems Xiao-Feng Pang, Yuan-Ping Feng, 2005 In the history of physics and science quantum mechanics has served as the foundation of modern science This book discusses the properties of microscopic particles in nonlinear systems principles of the nonlinear quantum mechanical theory and its applications in condensed matter polymers and biological systems The book is essentially composed of three parts The first part presents a review of linear quantum mechanics as well as theoretical and experimental fundamentals that establish the nonlinear quantum mechanical theory The theory itself and its essential features are covered in the second part In the final part extensive applications of this theory in physics biology and polymer are introduced The whole volume forms a complete system of nonlinear quantum mechanics The book is intended for

researchers graduate students as well as upper level undergraduates **Hydrogen Bonding - New Insights** Slawomir Grabowski, 2006-10-07 Hydrogen Bonding New Insights is an extensive text which takes numerous examples from experimental studies and uses these to illustrate theoretical investigations to allow a greater understanding of hydrogen bonding phenomenon The most important topics in recent studies are considered including Intra molecular H bonds Differences between H bond and van der Waals interactions from one side and covalent bonds from the other Bader theory to analyze H bonding Influence of weak H bonds upon structure and function of biological molecules H bonds in crystal structures With contributions from some of the foremost experts in this field this volume provides an invaluable resource for all members of the academic community looking for a comprehensive text on hydrogen bonding It will be of particular interest to physical and theoretical chemists spectroscopists crystallographers and those involved with chemical physics

Molecular simulation of proton transfer in hydrogen bonded systems Janez Mavri, 2003 *Hydrogen Bonding* Steve Scheiner, 1997 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

Deuterium and Shift Calculation, 2012-12-06 In 1931 Vrey Brickwedde and Murphy discovered the hydrogen isotope deuterium The isotopic enrichment was found to arise from the fact that the electrolysis of light water is faster than of heavy water 1 2 This success showed that although different isotopes of an element behave identically from a chemical standpoint the different isotopic masses nevertheless lead to both isotope effects on equilibrium as well as on rate constants of chemical reactions Soon ratios of equilibrium constants of isotopic reactions were called equilibrium isotope effects EIE ratios of isotopic rate constants kinetic isotope effects KIE Isotope effects have been found to be especially large for those elements which are directly involved in bond breaking and bond formation during the reaction studied 3 Such effects are therefore referred to as primary Isotopic substitution in atomic sites which maintain all chemical bonds with their neighbors during the reaction of interest leads then only to smaller secondary isotope effects Because of the unique mass relation between the different hydrogen isotopes hydrogen deuterium isotope effects are particularly large and have attracted most attention The largest contributions to these effects arise from changes in the vibrational frequencies of the reactants The theory of equilibrium isotope effects has been founded by Vrey 4 and Bigeleisen 5 6 and has widely been accepted 3 **Ab Initio**

Direct Dynamics Studies of Proton Transfer Reactions in Hydrogen Bonded Systems Robert L. Bell, 1997

Hydrogen Bond Research Peter Schuster, Werner Mikenda, 2012-12-06 Seven review articles and original papers provide a representative overview of the research work done in hydrogen bond research at Austrian universities. The topics covered by the contributions are state of the art of understanding hydrogen bonding in biopolymers, recent NMR techniques for studying hydrogen bonding in aqueous solutions, intramolecular hydrogen bonding and proton transfer in a class of Mannich bases derived from substituted phenols and naphthols, competition between intramolecular hydrogen bonds in ortho-disubstituted phenols, molecular dynamic simulations on proton transfer in 5,8-dihydroxynaphthoquinone and in the formic acid dimer, accurate calculations of the intermolecular interactions in cyanoacetylene dimers, correlation between OH...O bond distances and OH stretching frequencies as derived from structural and spectroscopic data of minerals.

Understanding Hydrogen Bonds Sławomir J. Grabowski, 2020-11-13 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 hydrogen 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-Parinello 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.

Computational Molecular Biology J. Leszczynski, 1999-06-10 This book covers applications of computational techniques to biological problems. These techniques are based by an ever growing number of researchers with different scientific backgrounds: biologists, chemists and physicists. The rapid development of molecular biology in recent years has been mirrored by the rapid development of computer hardware and software. This has resulted in the development of sophisticated computational techniques and a wide range of computer simulations involving such methods. Among the areas where progress has been profound is in the modeling of DNA structure and function, the understanding at a molecular level of the role of solvents in biological phenomena, the calculation of the properties of molecular associations in aqueous solutions, computationally assisted drug design, the prediction of protein structure and protein-DNA recognition, to mention just a few examples. This volume comprises a balanced blend of contributions covering such topics. They reveal the details of

computational approaches designed for biomolecules and provide extensive illustrations of current applications of modern techniques. A broad group of readers ranging from beginning graduate students to molecular biology professionals should be able to find useful contributions in this selection of reviews.

Quantum Biochemistry Chérif F. Matta, 2010-01-14 Divided into five major parts, the two volumes of this ready reference cover the tailoring of theoretical methods for biochemical computations as well as the many kinds of biomolecules, reaction and transition state elucidation, conformational flexibility, determination, and drug design. Throughout the chapters, gradually build up from introductory level to comprehensive reviews of the latest research and include all important compound classes such as DNA, RNA, enzymes, vitamins, and heterocyclic compounds. The result is in-depth and vital knowledge for both readers already working in the field as well as those entering it. Includes contributions by Prof. Ada Yonath, Nobel Prize in Chemistry 2009 and Prof. Jerome Karle, Nobel Prize in Chemistry 1985.

Isotope Effects In Chemistry and Biology Amnon Kohen, Hans-Heinrich Limbach, 2005-11-01 The field of isotope effects has expanded exponentially in the last decade and researchers are finding isotopes increasingly useful in their studies. Bringing literature on the subject up to date, *Isotope Effects in Chemistry and Biology* covers current principles, methods, and a broad range of applications of isotope effects in the physical biological sciences.

Quantum Systems in Chemistry and Physics. Trends in Methods and Applications R. McWeeny, Jean Maruani, Y.G. Smeyers, S. Wilson, 1998-01-31 *Quantum Systems in Chemistry and Physics* contains a refereed selection of the papers presented at the first European Workshop on this subject held at San Miniato near Pisa, Italy, in April 1996. The Workshop brought together leading experts in theoretical chemistry and molecular physics with an interest in the quantum mechanical many-body problem. This volume provides an insight into the latest research in this increasingly important field. Throughout the Workshop, the emphasis was on innovative theory and conceptual developments rather than on computational implementation. The various contributions presented reflect this emphasis and embrace topics such as density matrices and density functional theory, relativistic formulations, electron correlation, valence theory, nuclear motion, response theory, condensed matter, and chemical reactions. Audience: The volume will be of interest to those working in the molecular sciences and to theoretical chemists and molecular physicists in particular.

New Trends in Quantum Systems in Chemistry and Physics J. Maruani, Christian Minot, R. McWeeny, Y.G. Smeyers, Stephen Wilson, 2006-04-11 These two volumes collect thirty-eight selected papers from the scientific contributions presented at the Fourth European Workshop on Quantum Systems in Chemistry and Physics (QSCP IV) held in Marly le Roi, France, in April 22-27, 1999. A total of one hundred and fifteen scientists attended the workshop: 99 from Europe and 16 from the rest of the world. They discussed the state of the art, new trends, and future evolution of the methods and applications. The workshop was held in the old town of Marly le Roi, which lies to the West of Paris between the historic centres of Saint Germain en Laye and Versailles. Participants were housed at the National Youth Institute where over sixty lectures were given by leading members of the scientific community; in addition, over sixty posters were presented in two very animated

sessions We are grateful to the oral speakers and to the poster p senters for making the workshop such an stimulating experience The social programme was also memorable and notjust for the closing banquet which was held at the French Senate House We are sure that participants will long remember their visit to the Mus e des Antiquit s Nationales created by Napoleon III at the birthplace ofLouis XIV this museum boasts one ofthe world finest collections ofarcheological artifacts The Marly le Roi workshop followed the format established at the three previous meetings organized by Prof *Molecular Aspects of Biotechnology: Computational Models and Theories* Juan Bertrán,2012-12-06 Although biotechnology emerged from the genetic engineering revolution of the 70s the knowledge of the structure of genes revealed its molecular aspects Molecular biotechnology is a multidisciplinary domain of research in which experiments simulations and theories interact At present the huge increase in computer power allows us to carry out numerical simulations of biochemical systems However a fundamental question appears concerning the sophistication of the model utilized to capture the main features of biomolecules and biochemical processes In the present book a group of leading specialists in molecular biotechnology provides an answer to this question This book is thus an excellent tool for those researchers wishing to know the state of the art in this domain The book spans the range from molecular conformations through protein folding and from chemical reactivity through enzymatic action Furthermore it formulates recommendations for future research in molecular biotechnology

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