

An Introduction to Hydrogen Bonding



George A. Jeffrey

An Introduction To Hydrogen Bonding Topics In Physical Chemistry

Paolo Facci



An Introduction To Hydrogen Bonding Topics In Physical Chemistry:

An Introduction to Hydrogen Bonding George A. Jeffrey, 1997 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

Modern Physical Organic Chemistry Eric V. Anslyn, Dennis A. Dougherty, 2006 Making explicit the connections between physical organic chemistry and critical fields such as organometallic chemistry materials chemistry bioorganic chemistry and biochemistry this book escorts the reader into an area that has been thoroughly updated in recent times

Hydrogen Bonding Steve Scheiner, 1997-09-04 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

Spectroscopy and Computation of Hydrogen-Bonded Systems Marek J. Wójcik, Yukihiro Ozaki, 2022-12-13 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

Intermolecular and Surface Forces Jacob N. Israelachvili, 2011-07-22 *Intermolecular and Surface Forces* describes the role of various intermolecular and interparticle forces in determining the properties of simple systems such as gases liquids and solids with a special focus on more complex colloidal polymeric and biological systems The book provides a thorough foundation in theories and concepts of intermolecular forces allowing researchers and students to recognize which forces are important in any particular system as well as how to control these forces This third edition is expanded into three sections and contains five new chapters over the previous edition Starts from the basics and builds up to more complex systems Covers all aspects of intermolecular and interparticle forces both at the fundamental and applied levels Multidisciplinary approach bringing together and unifying phenomena from different fields This new edition has an expanded Part III and new chapters on non equilibrium dynamic interactions and tribology friction forces

Descriptive Inorganic Chemistry James E. House, Kathleen A. House, 2010-09-22 *Descriptive Inorganic Chemistry* Second Edition covers the synthesis reactions and properties of elements and inorganic compounds for courses in descriptive inorganic chemistry This updated version includes expanded coverage of chemical bonding and enhanced treatment of Buckminster Fullerenes and incorporates new industrial applications matched to key topics in the text It is suitable for the one semester ACS recommended course or as a supplement in general chemistry courses Ideal for majors and non majors the book incorporates rich graphs and diagrams to enhance the content and maximize learning Includes expanded coverage of chemical bonding and enhanced treatment of Buckminster Fullerenes Incorporates new industrial applications matched to key topics in the text

Modeling Solvent Environments Michael Feig, 2009-12-09 A comprehensive view of the current methods for modeling solvent environments with contributions from the leading researchers in the field Throughout the emphasis is placed on the application of such models in simulation studies of biological processes although the coverage is sufficiently broad to extend to other systems as well As such this monograph treats a full range of topics from statistical mechanics based approaches to popular mean field formalisms coarse grained solvent models more established explicit fully atomic solvent models and recent advances in applying ab initio methods for modeling solvent properties

Chemical Bonding in Crystals and Their Properties Anna V. Vologzhanina, Yulia V. Nelyubina, 2020-06-16 Unravelling an intricate network of interatomic interactions and their relations to different behaviors of chemical compounds is key to the successful design of new materials for both existing and novel applications

from medicine to innovative concepts of molecular electronics and spintronics X ray crystallography has proven to be very helpful in addressing many important chemical problems in modern materials science and biosciences Intertwined with computational techniques it provides insights into the nature of chemical bonding and the physicochemical properties including optical magnetic electrical mechanical and others of crystalline materials otherwise accessible by experimental techniques that are not so readily available to chemists In addition to the advanced approaches in charge density analysis made possible by X ray diffraction the information collected over the years through this technique which is easily mined from huge databases has tremendous use in the design of new materials for medicine gas storage and separation applications as well as for electronic devices This Special Issue contains two reviews and five articles that cover very different aspects of composition structure and structure property relations identified by X ray diffraction and complementary techniques from conventional IR and Raman spectroscopies to cutting edge quantum chemical calculations and their use in crystal engineering and materials science

An Introduction to Nonlinear Chemical Dynamics Irving R. Epstein, John A. Pojman, 1998-10-22 Assuming no more than an undergraduate knowledge of chemistry the authors take the reader through the necessary mathematical and theoretical background of oscillating reactions chaos and chemical waves to advanced topics of current research interest in chemical systems

Biomolecular Electronics Paolo Facci, 2014-04-03 Biomolecular Electronics the electrical control of biological phenomena is a scientific challenge that once fully realized will find a wide range of applications from electronics and computing to medicine and therapeutic techniques This new arena of biomolecular electronics is approached using familiar concepts from many areas such as electrochemistry device electronics and some mechanisms of gene expression level control Practical techniques are explored by which electrical and electronic means can be used to control biological reactions and processes Also the current and future applications for this new and expanding field are discussed This book is aimed at scientists and engineers involved in both research and commercial applications across fields including bioelectronics bionanotechnology electrochemistry and nanomedicine providing a state of the art survey of what's going on at the boundary between biology and electronic technology at the micro and nano scales along with a suggestive insight into future possible developments Demystifies the science and applications of electrically driven biological reactions Explains how the techniques of bioelectronics and electrochemistry can be deployed as biological control technologies Provides applications information for diverse areas from bio electrochemistry to electrical control of gene expression levels

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