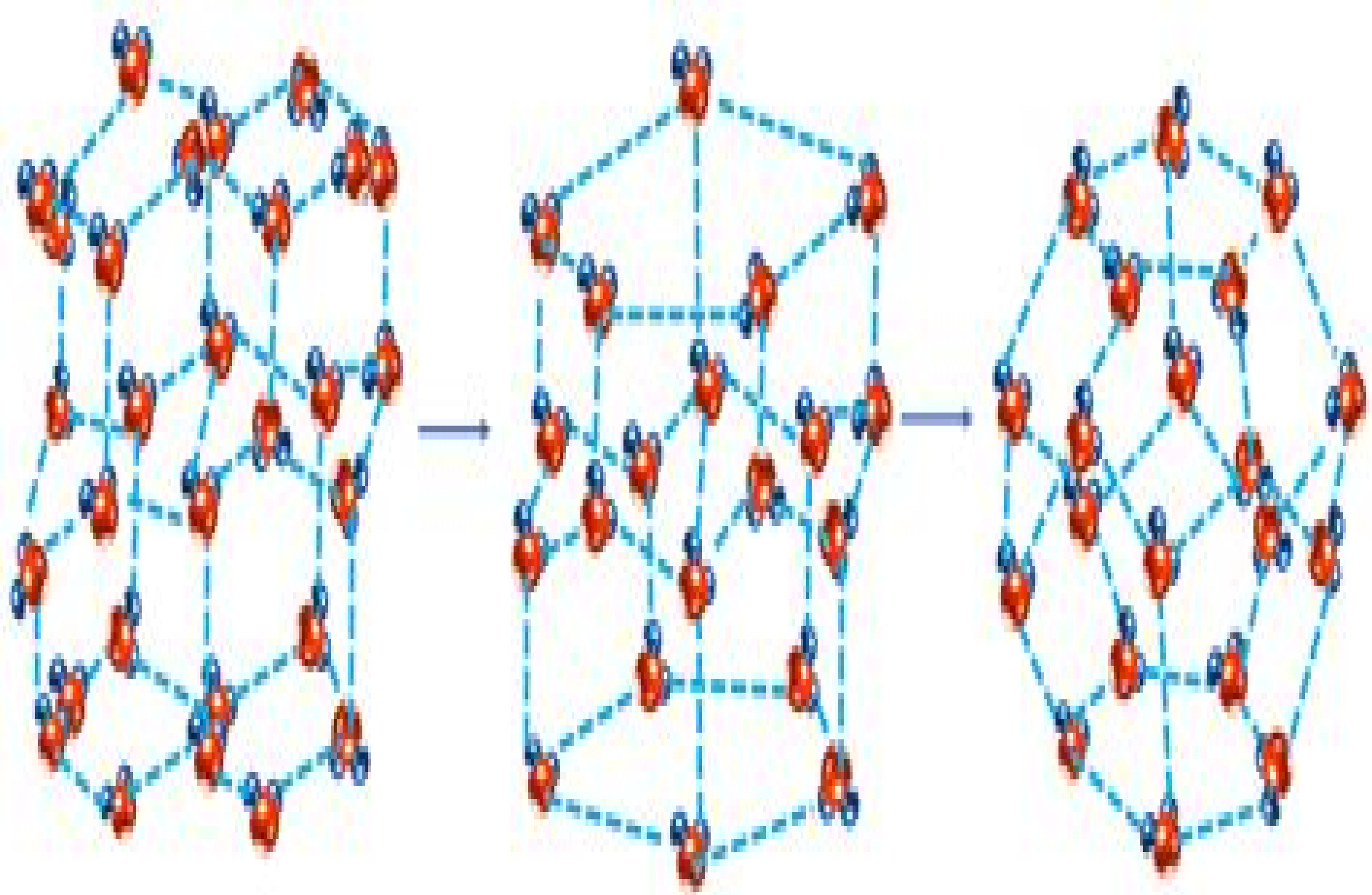




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Structure of Molecules and Internal Rotation San'ichirō Mizushima,1954 **Structure Of Molecules And Internal Rotation** San-Ichiro Mizushima,2021-09-09 This work has been selected by scholars as being culturally important and is part of the knowledge base of civilization as we know it This work is in the public domain in the United States of America and possibly other nations Within the United States you may freely copy and distribute this work as no entity individual or corporate has a copyright on the body of the work Scholars believe and we concur that this work is important enough to be preserved reproduced and made generally available to the public To ensure a quality reading experience this work has been proofread and republished using a format that seamlessly blends the original graphical elements with text in an easy to read typeface We appreciate your support of the preservation process and thank you for being an important part of keeping this knowledge alive and relevant Equilibrium Structure of Free Molecules Natalja Vogt,Jean Demaison,2023-12-06 The properties of chemical pharmaceutical and biological compounds depend mainly on their molecular structure whose determination is of fundamental interest This book examines and systematizes more than three hundred striking structural determinations of free molecules Featuring high quality structural data and presenting modern techniques of their determinations by quantum chemistry high resolution spectroscopy and electron diffraction the book is an indispensable resource for graduate students and professional scientists specializing in structural chemistry and other related fields **Structure of Molecules and Internal Rotation** San-Ichiro Mizushima,2013-10-22 Structure of Molecules and Internal Rotation reviews early studies on dihalogenoethanes This book is organized into two parts encompassing 8 chapters that evaluate the Raman effect in ethane derivatives the energy difference between rotational isomers and the infrared absorption of ethane derivatives Some of the topics covered in the book are the potential barrier to internal rotation nature of the hindering potential entropy difference between the rotational isomers internal rotation in butane pentane and hexane and internal rotation in long chain n paraffins Other chapters deal with the configuration of a polypeptide chain as well as the sum rule and the product rule for rotational isomers The normal vibrations of the 1 2 dihalogenoethanes are presented The last chapters are devoted to the examination of the Raman effect dielectric constant and electron diffraction The book can provide useful information to chemists physicists students and researchers Introduction to Chemical Structure Donald Cotter,2020-08-01 Rotational Spectra and Molecular Structure James E. Wollrab,2013-10-22 Physical Chemistry A Series of Monographs Rotational Spectra and Molecular Structure covers the energy levels and rotational transitions This book is divided into nine chapters that evaluate the rigid asymmetric top molecules and the nuclear spin statistics for asymmetric tops Some of the topics covered in the book are the asymmetric rotor functions rotational transition intensities classes of molecules nuclear spin statistics for linear molecules and symmetric tops and classical appearance of centrifugal and coriolis forces Other chapters deal with the energy levels and effects of centrifugal distortion as well as the

internuclear distance and moments of inertia The discussion then shifts to the coriolis coupling effects on rotational constants and the perturbation treatment of vibration rotational Hamiltonian The last chapter is devoted to the examination of origin of the quadrupole interaction The book can provide useful information to chemists physicists electrical engineers students and researchers

Structures and Conformations of Non-Rigid Molecules J. Laane, Marwan Dakkouri, Ben van der Veken, Heinz Oberhammer, 2012-12-06 From the beginnings of modern chemistry molecular structure has been a lively area of research and speculation For more than half a century spectroscopy and other methods have been available to characterize the structures and shapes of molecules particularly those that are rigid However most molecules are at least to some degree non rigid and this non rigidity plays an important role in such diverse areas as biological activity energy transfer and chemical reactivity In addition the large amplitude vibrations present in non rigid molecules give rise to unusual low energy vibrational level patterns which have a dramatic effect on the thermodynamic properties of these systems Only in recent years has a coherent picture of the energetics and dynamics of the conformational changes inherent in non rigid and semi rigid molecules begun to emerge Advances have been made in a number of different experimental areas vibrational infrared and Raman spectroscopy rotational microwave spectroscopy electron diffraction and most recently laser techniques probing both the ground and excited electronic states Theoretically the proliferation of powerful computers coupled with scientific insight has allowed both empirical and ab initio methods to increase our understanding of the forces responsible for the structures and energies of non rigid systems The development of theory group theoretical methods and potential energy surfaces to understand the unique characteristics of the spectra of these floppy molecules has also been necessary to reach our present level of understanding The thirty chapters in this volume contributed by the key speakers at the Workshop are divided over the various areas Both vibrational and rotational spectroscopy have been effective at determining the potential energy surfaces for non rigid molecules often in a complementary manner Recent laser fluorescence work has extended these types of studies to electronic excited states Electronic diffraction methods provide radial distribution functions from which both molecular structures and compositions of conformational mixtures can be found Ab initio calculations have progressed substantially over the past few years and when carried out at a sufficiently high level can accurately reproduce or predict ahead of time experimental findings Much of the controversy of the ARW related to the question of when an ab initio is reliable Since the computer programs are readily available many poor calculations have been carried out However excellent results can be obtained from computations when properly done A similar situation exists for experimental analyses The complexities of non rigid molecules are many but major strides have been taken to understand their structures and conformational processes

Molecular Structure by Diffraction Methods L E Sutton, M R Truter, 2007-10-31 Specialist Periodical Reports provide systematic and detailed review coverage of progress in the major areas of chemical research Written by experts in their specialist fields the series creates a unique service for the active research chemist supplying

regular critical in depth accounts of progress in particular areas of chemistry For over 80 years the Royal Society of Chemistry and its predecessor the Chemical Society have been publishing reports charting developments in chemistry which originally took the form of Annual Reports However by 1967 the whole spectrum of chemistry could no longer be contained within one volume and the series Specialist Periodical Reports was born The Annual Reports themselves still existed but were divided into two and subsequently three volumes covering Inorganic Organic and Physical Chemistry For more general coverage of the highlights in chemistry they remain a must Since that time the SPR series has altered according to the fluctuating degree of activity in various fields of chemistry Some titles have remained unchanged while others have altered their emphasis along with their titles some have been combined under a new name whereas others have had to be discontinued The current list of Specialist Periodical Reports can be seen on the inside flap of this volume

Structure and Dynamics of Non-Rigid Molecular Systems

Y.G. Smeyers, 2012-12-06 This volume contains a selection of scientific papers related to the structure and dynamics of non rigid molecules This frontline topic was born a few decades ago when Longuet Higgins proposed his famous theory of Molecular Symmetry Groups Mol Phys 6 1962 457 Unfortunately since this early paper very few publications have been devoted to the study of non rigid molecules Let us mention some books which dedicate some chapters to them Induced Representations in Crystals and Molecules by S L Altmann Academic Publishers 1977 Molecular Symmetry and Spectroscopy by P R Bunker Academic Publishers 1979 and finally Large Amplitude Motion in Molecules Vols I and II by several authors Springer Verlag 1979 More recently an International Symposium on Non Rigid Molecules was held in Paris France from 1 7 July 1982 the proceedings of which were published in the volume entitled Symmetries and Properties of Non Rigid Molecules A Comprehensive Survey edited by J Maruani et al Elsevier 1983 Finally we should mention the very specialized work The Permutational Approach to Dynamic Stereochemistry by J Brocas et al McGraw Hill 1983 The purpose of this book is to fill in this information on the structure and dynamics of non rigid systems To this aim we have gathered a collection of recent papers written by the most qualified specialists in the world covering a large field from van der Waals molecules to inorganic complexes and organic polyrotor molecules as well as considering statistical and dynamic aspects

Structure Data of Free Polyatomic Molecules Natalja Vogt, Jürgen Vogt, 2020-01-02 This handbook presents structural data on free polyatomic molecules Since the structure of molecules defines the chemical physical and biological properties of matter this information is crucial for understanding explaining and predicting chemical reactions and biochemical processes developing new drugs and materials as well as studying interstellar media Covering the structural data published between 2009 and 2017 this book supplements the previous Landolt B r nstein volumes Structure Data of Free Polyatomic Molecules eds K Kuchitsu N Vogt M Tanimoto which included data from the literature published up to 2008 It systematizes and describes peculiarities of molecular structures for about 1000 compounds studied mainly by gas phase electron diffraction and rotational spectroscopy All structures are given in three dimensional representations

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