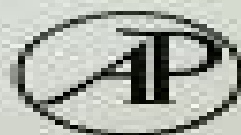


STRUCTURE OF MOLECULES and INTERNAL ROTATION

By

SAN-ICHIRO MIZUSHIMA

Professor of Physical Chemistry of the University of Tokyo



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Structure Of Molecules Internal Rotati

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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

A Study of Molecular Structure and Internal Rotation in Amides by Nuclear Magnetic Resonance Spectroscopy Lester Reinhardt Isbrandt, 1972 **Introduction to Chemical Structure** Donald Cotter, 2020-08-01

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 **Handbook of High-resolution Spectroscopy** Martin Quack, Frederic Merkt, 2011-09-26 The field of High Resolution Spectroscopy has been considerably extended and even redefined in some areas Combining the

knowledge of spectroscopy laser technology chemical computation and experiments Handbook of High Resolution Spectroscopy provides a comprehensive survey of the whole field as it presents itself today with emphasis on the recent developments This essential handbook for advanced research students graduate students and researchers takes a systematic approach through the range of wavelengths and includes the latest advances in experiment and theory that will help and guide future applications The first comprehensive survey in high resolution molecular spectroscopy for over 15 years Brings together the knowledge of spectroscopy laser technology chemical computation and experiments Brings the reader up to date with the many advances that have been made in recent times Takes the reader through the range of wavelengths covering all possible techniques such as Microwave Spectroscopy Infrared Spectroscopy Raman Spectroscopy VIS UV and VUV Combines theoretical computational and experimental aspects Has numerous applications in a wide range of scientific domains Edited by two leaders in this field Provides an overview of rotational vibration electronic and photoelectron spectroscopy Volume 1 Introduction Fundamentals of Molecular Spectroscopy Volume 2 High Resolution Molecular Spectroscopy Methods and Results Volume 3 Special Methods Applications *Frontiers and Advances in Molecular Spectroscopy* Jaan Laane, 2017-11-13 *Frontiers and Advances in Molecular Spectroscopy* once again brings together the most eminent scientists from around the world to describe their work at the cutting edge of molecular spectroscopy Much of what we know about atoms molecules and the nature of matter has been obtained using spectroscopy over the last one hundred years or so Going far beyond the topics discussed in Jaan Laane's earlier book on the subject these chapters describe new methodologies and applications instrumental developments and theory which are taking spectroscopy into still new frontiers The robust range of topics once again demonstrates the wide utility of spectroscopic techniques New topics include ultrafast spectroscopy of the transition state SERS far uv spectroscopy femtosecond coherent anti Stokes Raman spectroscopy high resolution laser induced fluorescence spectroscopy Raman spectroscopy and biosensors vibrational optical activity ultrafast two dimensional spectroscopy biology with x ray lasers isomerization dynamics and hydrogen bonding single molecule imaging spectra of intermediates matrix isolation spectroscopy and more Covers spectroscopic investigations on the cutting edge of science Written and edited by leading experts in their respective fields Allows researchers to access a broad range of essential modern spectroscopy content from a single source rather than wading through hundreds of scattered journal articles **Encyclopedia of Spectroscopy and Spectrometry**, 2016-09-22 This third edition of the Encyclopedia of Spectroscopy and Spectrometry Three Volume Set provides authoritative and comprehensive coverage of all aspects of spectroscopy and closely related subjects that use the same fundamental principles including mass spectrometry imaging techniques and applications It includes the history theoretical background details of instrumentation and technology and current applications of the key areas of spectroscopy The new edition will include over 80 new articles across the field These will complement those from the previous edition which have been brought up to date to reflect the latest trends in the field

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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 *NBS Special Publication* ,1978

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