Conformational Analysis Of Molecules In Excited States

MUHAMMAD KINGSTON

Molecular Similarity in Drug Design John Wiley & Sons
''Excellent and very timely....It will undoubtedly become a standard reference for the application of circular dichroism (CD) to biomolecules.'' --- Quarterly Review of Biology, March 1997 ''[T]estament to the book's utility is the fact that during the course of my review I had to 'rescue' it from the desks of graduate students on an almost daily basis. In summary, this is a great book.'' --- American Scientist ''Well documented chapters provide a very good insight into the problems surrounding the conformation of biomacromolecules...An indispensible source of information.'' --- Nahrung, 42(2), 1998 Renowned experts present the first state-of-the-art description of circular dichroism spectroscopy (CD). Chapters present in-depth discussions of the history of the field, the theory of CD for application to globular proteins, membrane proteins, peptides, nucleic acids and their interactions, carbohydrates, and instrumentation. Discussions also feature new techniques using synchrotron radiation, vibrational Raman optical activity, and vibrational CD. More than 250 illustrations supplement the text.
Structure Correlation John Wiley & Sons
The goal of these two volumes is to help fill the gap between theory and experiment in membrane science. This is the only work available today which covers the domain of computer-aided conformational analyses of membranes. Written in a detailed, yet comprehensive manner, this book uses the semi-empirical approach as a way to give a molecular description of the membrane structure in organized systems. This interesting work establishes the validity and quality of the prediction by making a permanent comparison with the experimental data. This reference aims to use this comparison to open a new avenue in the molecular description of the biological membrane. Those involved with biochemistry, biophysics, pharmacology, and biology will find these volumes interesting and informative.
The Conformational Universe of Proteins and Peptides Springer Science & Business Media
The Nuclear Overhauser Effect in Structural and Conformational Analysis, Second Edition, uniquely explains the NOE in detail, making it an indispensable resource for the novice as well as the experienced NMR researcher.
Methods in Protein Structure and Stability Analysis: Conformational stability, size, shape, and surface of protein molecules Elsevier
The most concise and streamlined textbook available on organic chemistry for the pharmacy student Organic Chemistry for Pharmacy is a textbook written specifically for the students taking the required Organic/Medical Pharmacy course. Using a building-block approach, the book delivers a basic, yet thorough discussion of the mode of action, therapeutic applications, and limitations of various pharmaceutical agents. Organic Chemistry for Pharmacy is especially written for students who have a limited background in chemistry. In order to make the learning/teaching experience as efficient as possible, Organic Chemistry for Pharmacy includes outstanding pedagogical features such as chapter outlines, chapter summaries, boxed “take away points”, quick-reference tables, and problems within each chapter. The focus and presentation of this text is particularly suited for Organic/Medical Pharmacy courses which are weighted heavily towards Organic, rather than Medical Pharmacy.
Recent Experimental and Computational Advances in Molecular Spectroscopy CRC Press
A unique look at some of the hottest topics in photophysics and photochemistry today The study of molecules in excited states has exploded over the past decade, providing new insights into conformational changes in organic molecules and opening up research opportunities for scientists and professionals in chemistry, physics, biology, medicine, and materials engineering. Using conformational analysis as a unifying concept, this important new work provides readers with a cohesive and cutting-edge overview of this fascinating and challenging field. From conformational changes accompanying photoinduced electron transfer to elementary photophysical and photochemical processes in living systems, the most representative and challenging topics are carefully gleaned from the vast literature, highlighting major conceptual problems along with the relevant experimental techniques. Authoritative, detailed contributions from both experimentalists and theoreticians include coverage of: * Conformational changes in intramolecular excited state electron transfer * Conformational aspects of excited state proton transfer * The novel topic of solute-solvent friction in chemical reactions * Mechanisms and structural aspects of exciplex formations * Conformational aspects of organic photochemistry * Calculations of excited state conformational properties
Conformations Wiley-Interscience
Conformational Analysis of Polymers Comprehensive resource focusing on theoretical methods and experimental techniques to analyze physical polymer chemistry Connecting varied issues to demonstrate the impact on areas like biodegradability, environmental friendliness, structure-property relationship, and molecular design, Conformational Analysis of Polymers introduces theoretical methods and experimental techniques to analyze physical polymer chemistry. Opening with a description of fundamental concepts and then describing the conformational characteristics of various polymers, including different heteroatoms and chemical species, the text continues onto the applications of density functional theory (DFT) to polymer crystals and structure-property relationships. The book concludes by bringing these issues together to demonstrate their practical impact on different areas of the field. Various methods and techniques, including DFT, statistical mechanics, NMR, spectroscopy, and molecular orbital theory, are also covered. Written by a highly qualified author, Conformational Analysis of Polymers explores sample topics such as: Fundamentals of polymer physical chemistry: stereochemistry of polymers, models for polymeric chains, Flory-Huggins theory, and rubber elasticity Quantum chemistry for polymers: ab initio molecular orbital theory, DFT, NMR parameters, and periodic DFT of polymer crystals Statistical mechanics of polymeric chains: basic rotational isomeric state (RIS) scheme, refined RIS method, inversional-rotational isomeric state method, and probability theory for RIS scheme Experimental techniques: NMR and scattering methods Providing a timely update to the field of chain conformations of synthetic polymers and connecting fundamental theoretical approaches, experimental techniques, and case study applications; Conformational Analysis of Polymers is an essential resource for polymer chemists, physicists, and material scientists, industrial engineers who synthesize and process polymers, and academic researchers.
The Organic Chemistry of Medicinal Agents John Wiley & Sons
Both molecular spectroscopy and computational chemistry have witnessed rapid significant progresses in recent years. On the one hand, it is nowadays possible to compute, to quite a reasonable degree of accuracy, almost all fundamental spectroscopic properties for small molecular systems. The theoretical approach is now properly considered to be of fundamental importance in attaining a high degree of understanding of spectroscopic information. Moreover, it may be also a great help in designing and planning experiments. On the other hand, new and very powerful experimental techniques have been developed. This book combines an advanced teaching standpoint with an emphasis on the interplay between theoretical and experimental molecular spectroscopy. It covers a wide range of topics (such as molecular dynamics and reactivity, conformational analysis, hydrogen bonding and solvent effects, spectroscopy of excited states, complex spectra interpretation and simulation, software development and biochemical applications of molecular spectroscopy) and considers a large variety of molecular spectroscopic techniques, either from an experimental or from a theoretical perspective. (short text) This book combines an advanced teaching standpoint with an emphasis on the interplay between theoretical and experimental molecular spectroscopy. It

covers a wide range of topics (such as molecular dynamics and reactivity, conformational analysis, hydrogen bonding and solvent effects, spectroscopy of excited states, complex spectra interpretation and simulation, software development and biochemical applications of molecular spectroscopy) and considers a large variety of molecular spectroscopic techniques either from an experimental or from a theoretical perspective.
The Conformational Analysis of Small, Flexible Molecules Using NMR of Liquid Crytalline Solutions Wiley-VCH
I get by with a little help from my friends The Beatles: Sgt. Pepper This book should have been in Danish. Any decent person must be able to express himself in his mother's tongue, also when expounding scientific ideas and results. Had I stuck to this ideal, the book would have been read by very few people, and, indeed, appreciated by even fewer. Having it publU' ished in English gives me a chance to fulfill one ambition: to be read and judged by the international scientific community. Another reason is that the majority of my professional friends are regrettably unread in Danish, just as I am in Hebrew, Finnish and even Italian. I want to deprive them of the most obvious excuse for not reading my opus. Like a man I admired, I will first of all thank my wife. In his autobiography, Meir Weisgal, then President of the Weizmann InstiU' tute of SCience, wrote about his wife: "In addition to her natural endowments - which are considerable - she was a more than competent part-tim~ secretary." He wrote on, and so shall I. The book has been edited by my wife. So if the reader finds the layout pleasant as, in actual fact, I myself do, Birgit is to be praised. If there are blemishes, I am to be blamed for not having caught them
Conformational Analysis of Cyclohexenes, Cyclohexadienes, and Related Hydroaromatic Compounds John Wiley & Sons
Stereochemistry of Organic Compounds The first fully referenced, comprehensive book on this subject in more than thirty years, Stereochemistry of Organic Compounds contains up-to-date coverage and insightful exposition of all important new concepts, developments, and tools in the rapidly advancing field of stereochemistry, including: * Asymmetric and diastereoselective synthesis * Conformational analysis * Properties of enantiomers and racemates * Separation and analysis of enantiomers and diastereoisomers * Developments in spectroscopy (including NMR), chromatography, and molecular mechanics as applied to stereochemistry * Prostereoisomerism * Conceptual foundations of stereochemistry, including terminology and symmetry concepts * Chiroptical properties Written by the leading authorities in the field, the text includes more than 4,000 references, 1,000 illustrations, and a glossary of stereochemical terms.
Conformational Analysis of Molecules in Excited States McGraw Hill Professional
This text will give the reader a firm understanding of all aspects of carbohydrate conformation by describing and explaining the importance of interactions between carbohydrates and interactions of carbohydrates with proteins, nucleic acids or any other macromolecule., The authors have gathered a wealth of information on carbohydrate structures, different methods of conformational analysis, the role of carbohydrates as recognition molecules in biological systems and their industrial applications., Whether you are a student, teacher or a basic researcher, this text book is a ‘one-stop’ source of current information on carbohydrate conformation and the potential use of conformational properties in industry and also of their crucial role in important biological events such as cell-cell interaction, cell adhesion, cellular signaling mechanism.
The Conformational Analysis of Heterocyclic Compounds John Wiley & Sons
Unter Zirkulardichroismus (CD) versteht man die spezifisch unterschiedliche Absorption von links- und rechtszirkular polarisiertem Licht durch bestimmte Moleküle. CD-Effekte lassen sich in Abhängigkeit von der Wellenlänge messen und spektroskopisch auswerten; sie geben beispielsweise Auskunft über die Konformation organischer Verbindungen. Dieses Buch richtet sich an den organischen Chemiker, der mit den Grundprinzipien der Stereochemie vertraut ist, und erläutert die Anwendung der CD-Spektroskopie zur Konformationsanalyse ausführlich und verständlich. (06/00)
The Nuclear Overhauser Effect in Structural and Conformational Analysis Springer Science & Business Media
Viele Bücher über organische Zusammensetzungen behandeln die Stereochemie, schenken aber der räumlichen Struktur der organischen Moleküle, vor allem der weniger gebräuchlichen, kaum Beachtung. Diese Monographie stellt nun ein umfassendes Werk zur organischen Struktur und der Konformationsanalyse dar. Das Interesse des Autors an der Formenvielfalt der organischen Moleküle spiegelt sich besonders intensiv in der Betrachtung der Molekülordnung wider, die in organisch chemischen und biologischen Systemen von großer Bedeutung ist. Der neue Band in der Reihe 'Methods in Stereochemical Analysis' stellt vor allem diese Bedeutung der Molekülgestalt und die Einwirkung theoretischer Studien und synthetischer Chemie zu diesem Themenkomplex in den Vordergrund.
Modern Conformational Analysis Wiley-VCH
Conformational Analysis: Scope and Present Limitations contains the proceedings of the Brussels International Symposium on Conformational Analysis held in Brussels, Belgium, in September 1969. The papers focus on the theoretical aspects and applications of conformational analysis, such as those concerning the aliphatic and especially the cyclic series. Topics covered include the geometry of five-membered rings; conformational transmission in steroids; conformational aspects of N-quaternization; and applications of nuclear magnetic resonance spectrometry in conformational studies of cyclohexane derivatives. This book is comprised of 20 chapters and begins with a discussion on the conformational aspects of some five-membered ring compounds based mainly on observed (diffraction methods) and calculated torsional angles. The reader is then introduced to nuclear magnetic resonance studies of the conformations and conformational barriers in cyclic molecules; conformational studies of six-membered heterocycles; conformational transmission in steroids; and solvolytic cyclizations involving double bonds. The remaining chapters explore the conformational analysis of methylcyclohexane, cyclohexane systems, and carbonium ions; conformations of membrane-active cyclodepsipeptides; energetics of isomeric transition states and competitive reaction pathways in conformational analysis; and conformational aspects of the reaction of the 1-methylcyclodecane-l,6-diols with acid. This monograph will be of interest to organic chemists.
Conformational Analysis Wiley-Blackwell
The goal of these two volumes is to help fill the gap between theory and experiment in membrane science. This is the only work available today which covers the domain of computer-aided conformational analyses of membranes. Written in a detailed, yet comprehensive manner, this book uses the semi-empirical approach as a way to give a molecular description of the membrane structure in organized systems. This interesting work establishes the validity and quality of the prediction by making a permanent comparison with the experimental data. This reference aims to use this comparison to open a new avenue in the molecular description of the biological membrane. Those involved with biochemistry, biophysics, pharmacology, and biology will find these volumes interesting and informative.
Protein Structure and Function CRC Press
Written by experienced experts in molecular modeling, this books describes the basics to the extent that is necessary if one wants to be able to reliably judge the results from molecular modeling calculations. Its main objective is the description of the various pitfalls to be avoided. Without unnecessary overhead it leads the reader from simple calculations on small molecules to the modeling of proteins and other relevant biomolecules. A textbook for beginners as well as an invaluable reference for all those dealing with molecular modeling in their daily work!
Conformational Analysis CRC Press
Molecular similarity searching is fast becoming a key tool in organic chemistry. In this book, the editor has brought together an international team of authors, each working at the forefront of this technology, providing a timely and concise overview of current research. The chapters focus principally on those methods which have reached sufficient maturity to be of immediate practical use in molecular design.
Conformation of Carbohydrates Wiley-VCH
This innovative book presents an original account of the principles of conformational theory. It has a strong focus on computational methodologies for conformational space exploration. By revisiting basic conformational conventions, considering experimental results which are often misinterpreted by organic chemists, and qualitatively analyzing the potential energy surface, the book helps non-experts to understand molecular flexibility at the level required in contemporary research.The book shows synthetic organic chemists how to perform successful conformational studies using widespread calculation packages ('click computational chemistry') instead of being misguided by textbook-based conformational analysis. The monograph actually offers to synthetic chemists a new research tool that can significantly upgrade their ability to predict, or at least explain, regioselectivity and stereoselectivity in their own reactions.
Conformational Behavior of Six-membered Rings CRC Press
Among the materials found in Nature’s many diverse living organisms or produced by human industry, those made from polymers are dominant. In Nature, they are not only dominant, but they are, as well, uniquely necessary to life. Conformations: Connecting the Chemical Structures and Material Behaviors of Polymers explores how the detailed chemical structures of polymers can be characterized, how their microstructural-dependent conformational preferences can be evaluated, and how these conformational preferences can be connected to the behaviors and properties of their materials. The authors examine the connections between the microstructures of polymers and the rich variety of physical properties they evidence. Detailed polymer architectures, including the molecular bonding and geometries of backbone and side-chain groups, monomer stereo- and regiosequences, comonomer sequences, and branching, are explicitly considered in the analysis of the conformational characteristics of polymers. This valuable reference provides practicing materials engineers as well as polymer and materials science students a means of understanding the differences in behaviors and properties of materials made from chemically distinct polymers. This knowledge can assist the reader design polymers with chemical structures that lead to their desired material behaviors and properties.
Structures and Conformations of Non-Rigid Molecules Elsevier
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.
Principles of Asymmetric Synthesis World Scientific
The goal of these two volumes is to help fill the gap between theory and experiment in membrane science. This is the only work available today which covers the domain of computer-aided conformational analyses of membranes. Written in a detailed, yet comprehensive manner, this book uses the semi-empirical approach as a way to give a molecular description of the membrane structure in organized systems. This interesting work establishes the validity and quality of the prediction by making a permanent comparison with the experimental data. This reference aims to use this comparison to open a new avenue in the molecular description of the biological membrane. Those involved with biochemistry, biophysics, pharmacology, and biology will find these volumes interesting and informative.