

Two-Dimensional NMR Spectroscopy

*Applications for Chemists
and Biochemists*

Second Edition

Edited by

William R. Croasmun
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Two Dimensional Nmr Spectroscopy Applications For Chemists And Biochemists Methods In Stereochemical Analysis

W. R. Croasmun



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Two-Dimensional Nmr Spectroscopy W. R. Croasmun, 1998-04-01 *Two-dimensional NMR Spectroscopy* William R. Croasmun, Robert M. K. Carlson, 1994 **Methods in stereochemical analysis**, 1987 **Two-Dimensional NMR Spectroscopy** W. R. Croasmun, Robert M. K. Carlson, 1996-12-17 This volume covers the new methodological advances in NMR spectroscopy that have been developed since the publication of the first edition These include indirect detection methods particularly proton detected carbon 13 spectra which have profoundly increased NMR sensitivities 3 and even higher dimensional NMR methods which have further increased spectral resolving and correlating power powerful new computer programs which assist in all phases of data analysis and ultimately make possible rigorous interpretations of complex 2D and higher dimensional NMR spectra using molecular mechanics and dynamics calculations and field gradient technology which makes it possible to acquire 2D and higher dimensional spectra of concentrated samples very rapidly greatly reducing experiment times This new edition retains the original format of the first edition with introductory chapters covering descriptions basic theoretical treatments and experimental aspects of the methods These are followed by applications chapters representing a broad sampling of important research areas and compound classes Crystal Structure Analysis for Chemists and Biologists Jenny P. Glusker, Mitchell Lewis, Miriam Rossi, 1996-12-17 The fields of structural chemistry and biochemistry have blossomed in the last seventy years since X ray diffraction was discovered in 1912 Dorothy Hodgkin who obtained a Nobel Prize in 1965 for her X ray diffraction work wrote a great advantage of X ray analysis as a method of chemical structure analysis is its power to show some totally unexpected and surprising structure with at the same time complete certainty The results of all X ray diffraction studies are used by chemists and buiochemists but these scientists need to be able to appreciate the significance and extent to which these results may be used A number of books written for practicing crystallographers cover the theory and applications of X ray diffraction but few are of real practical use to non specialists In Crystal Structure Analysis for Biologists and Chemists the general principles of crystal structure are presented in a highly readable way The book of Glusker who is internationally renowned provides good coverage of theory including data and understanding their significance **Organic Conformational Analysis and Stereochemistry from Circular Dichroism Spectroscopy** David A. Lightner, Jerome E. Gurst, 2000-03-31 A unique guide to variable temperature CD spectroscopy and its application in organic chemistry This timely original thought provoking work looks at organic stereochemistry from the perspective of circular dichroism CD using variable temperature CD spectroscopy to determine the conformation or absolute configuration of chiral molecules With an emphasis on the analysis of optically active ketones and the carbonyl chromophore the authors demonstrate the advantages of this highly sensitive spectroscopic tool for obtaining stereochemical information in diverse areas of organic chemistry biochemistry and medicinal

pharmaceutical chemistry They combine detailed examples of stereochemical analysis with clear thorough presentations correlating chiroptical data with molecular mechanics calculations as well as data from NMR spectroscopy and other spectroscopic techniques In addition they provide a systematic survey of the professional literature featuring an extraordinary collection of original CD spectra run at varying temperatures Coverage includes Chiroptical measurements CD and ORD Optical Rotatory Dispersion Conformational analysis of compounds ranging from simple cyclic ketones to polycyclics Conjugated and homoconjugated systems Stereochemistry of the carbon carbon double bond Stereochemistry from exciton coupling of two or more chromophores An interesting historical account of the development of stereochemical concepts

NMR in Organometallic Chemistry Paul S. Pregosin, 2013-07-26 The first and ultimate guide for anyone working in transition organometallic chemistry and related fields providing the background and practical guidance on how to efficiently work with routine research problems in NMR The book adopts a problem solving approach with many examples taken from recent literature to show readers how to interpret the data Perfect for PhD students postdocs and other newcomers in organometallic and inorganic chemistry as well as for organic chemists involved in transition metal catalysis

Two-dimensional NMR Spectroscopy Lionel Salem, 1987 **Two-Dimensional NMR Spectroscopy** Jan Schraml, Jon M. Bellama, 1988-06-28 New York John Wiley and Sons c 1988

NMR Applications in Biopolymers John W. Finley, Siegfried J. Schmidt, A.S. Serianni, 2012-12-06 Elucidating the structures of biopolymers as they exist in nature has long been a goal of biochemists and biologists Understanding how these substances interact with themselves other solutes and solvents can provide useful insights into many areas of biochemistry agriculture food science and medicine Knowledge of the structure of a protein or complex carbohydrate in its native form provides guidelines for the chemical or genetic modifications often desired to optimize these compounds to specific needs and applications For example in the pharmaceutical industry structure function relationships involving biopolymers are studied routinely as a means to design new drugs and improve their efficacies The tools to conduct structure investigations of biopolymers at the molecular level are limited in number Historically X ray crystallography has been the most attractive method to conduct studies of this type However X ray methods can only be applied to highly ordered crystalline materials thus obviating studies of solution dynamics that are often critical to attaining a global understanding of biopolymer behavior In recent years nuclear magnetic resonance NMR spectroscopy has evolved to become a powerful tool to probe the structures of biopolymers in solution and in the solid state NMR provides a means to study the dynamics of polymers in solution and to examine the effects of solute solvent and other factors on polymer behavior With the development of 2D and 3D forms of NMR spectroscopy it is now possible to assess the solution conformations of small proteins oligonucleotides and oligosaccharides

The CH/ π Interaction Motohiro Nishio, Minoru Hirota, Yoji Umezawa, 1998-06-10 A systematic exploration of the fascinating area of CH π interaction from the frontier of chemical research The CH π bond may be the weakest of the hydrogen bonds but it has been found to play

important roles in the physical chemical and biological properties of a variety of substances This book offers a complete overview of the experimental basis theoretical background and nature of the CH π interaction to facilitate a clearer common understanding of the interaction between CH bonds and π systems Featured topics include Evidence and methods of detection Quantum chemical treatment of CH π interaction Comparison with other types of weak molecular interactions Conformational consequences Chiroptical properties Selectivity in organic reactions Crystal structures of clathrates Inclusion compounds Interligand interactions in coordination chemistry Specific interactions in protein structures Prospects and possibilities for use in biochemistry and materials science The CH π Interaction makes an important contribution to the understanding of weak intermolecular forces and their potential value to the biochemical and pharmaceutical sciences It will be welcomed by physical and synthetic organic chemists structural chemists and pharmaceutical and biochemists

New Advances in Analytical Chemistry, Volume 3 Atta-ur Rahman, 2002-04-11 New Advances in Analytical Chemistry Volume 3 presents recent developments in various spectroscopic techniques such as NMR spectroscopy and mass spectroscopy in the form of comprehensive reviews written by leading authorities in the field With new and updated information the book is invaluable to both research students and postdoctoral workers w

Molecular Design and Modeling John Joseph Langone, 1991 Computer based design and modeling computational approaches and instrumental methods for elucidating molecular mechanisms of protein folding and ligand acceptor interactions are included in Volumes 202 and 203 as are genetic and chemical methods for the production of functional molecules including antibodies and antigens enzymes receptors nucleic acids and polysaccharides and drugs

Conformational Analysis of Molecules in Excited States Jacek Waluk, 2000-06-13 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

Molecular Structure and Biological Activity of Steroids Martin Bohl, 2018-01-18 Molecular Structure and Biological Activity of Steroids focuses on the identification of steroid structural features that

control particular biological effects Steroid geometry plays a critical role in steroid activity therefore the results of X ray crystallographic NMR spectroscopic and theoretical studies on structure activity relationships form an integral part of the book Well established observations and proposed models are presented summarizing knowledge of molecular features e g steroid backbone structures side chain constitutions substitution sites configurations hydrogen bonding patterns that can affect steroid action The book also provides overviews about recent progress in various frontier fields of steroid research including such areas as sex steroids glucocorticoids aromatase inhibitors vitamin D metabolites brassinosteroids neuromuscular blocking agents and cardiotonic steroids Molecular Structure and Biological Activity of Steroids is a must have resource for biochemists pharmacologists endocrinologists biophysicists and others actively involved in steroid research

The Biomarker Guide: Volume 1, Biomarkers and Isotopes in the Environment and Human History K. E. Peters, C. C. Walters, J. M. Moldowan, 2007-08-16 The second edition of The Biomarker Guide is a fully updated and expanded version of this essential reference Now in two volumes it provides a comprehensive account of the role that biomarker technology plays both in petroleum exploration and in understanding Earth history and processes Biomarkers and Isotopes in the Environment and Human History details the origins of biomarkers and introduces basic chemical principles relevant to their study It discusses analytical techniques and applications of biomarkers to environmental and archaeological problems The Biomarker Guide is an invaluable resource for geologists petroleum geochemists biogeochemists environmental scientists and archaeologists

Modern Conformational Analysis Helena Dodziuk, 1996-12-17 Most books on organic conformational deal with stereochemistry while neglecting the spatial structure of organic molecules especially the unusual ones This ambitious monograph presents a global view of organic structure and conformational analysis in a very readable style The author's fascination with the beauty and variety of shapes of organic molecules comes through in her description of the importance of molecular organization in organic chemical and biological systems the quantum foundations of molecular spatial structure molecular symmetry chirality and physical methods for studying molecular geometry She provides ample bases for the new trends in organic conformational chemistry including the application of Computer Assisted Molecular Design CAMD to organic synthesis

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Polysaccharides Severian Dumitriu, 1998-05-12 Offers comprehensive coverage of the structural characterization of polysaccharides emphasizing commercially available and potential exopolysaccharides as well

as new applications Presents the major chemical and physical properties of polysaccharides and derivatives **Fortschritte der Chemie organischer Naturstoffe / Progress in the Chemistry of Organic Natural Products** A. Andersen, S.B. Christensen, D. Deepak, G. Gäde, A. Khare, U.W. Smitt, S. Srivastav, 1997-05-28 The volumes of this classic series now referred to simply as Zechmeister after its founder L Zechmeister have appeared under the Springer Imprint ever since the series inauguration in 1938 The volumes contain contributions on various topics related to the origin distribution chemistry synthesis biochemistry function or use of various classes of naturally occurring substances ranging from small molecules to biopolymers Each contribution is written by a recognized authority in his field and provides a comprehensive and up to date review of the topic in question Addressed to biologists technologists and chemists alike the series can be used by the expert as a source of information and literature citations and by the non expert as a means of orientation in a rapidly developing discipline

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