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Nuclear Magnetic Resonance
Introduction to NMR Spectroscopy
Spin Dynamics
Introduction to Organic Spectroscopy
Essential Practical NMR for Organic Chemistry

ELLISON JOVANY

Phosphorus-31 NMR Spectroscopy
Springer Science & Business Media
This text is aimed at people who have some familiarity with high-resolution NMR and who wish to deepen their understanding of how NMR experiments actually ‘work’. This revised and updated edition takes the same approach as the highly-acclaimed first edition. The text concentrates on the description of commonly-used experiments and explains in detail the theory behind how such experiments work. The quantum mechanical tools needed to analyse pulse sequences are introduced set by step, but the approach is relatively informal with the emphasis on obtaining a good understanding of how the experiments actually work. The use of two-colour printing and a new larger format improves the readability of the text. In addition, a number of new topics have been introduced: How product operators can be extended to describe

experiments in AX2 and AX3 spin systems, thus making it possible to discuss the important APT, INEPT and DEPT experiments often used in carbon-13 NMR. Spin system analysis i.e. how shifts and couplings can be extracted from strongly-coupled (second-order) spectra. How the presence of chemically equivalent spins leads to spectral features which are somewhat unusual and possibly misleading, even at high magnetic fields. A discussion of chemical exchange effects has been introduced in order to help with the explanation of transverse relaxation. The double-quantum spectroscopy of a three-spin system is now considered in more detail. Reviews of the First Edition “For anyone wishing to know what really goes on in their NMR experiments, I would highly recommend this book” – Chemistry World “...I warmly recommend for budding NMR spectroscopists, or others who wish to deepen their understanding of elementary NMR theory or theoretical tools” – Magnetic Resonance in Chemistry

Nuclear Magnetic Resonance Spectroscopy Springer

Nuclear magnetic resonance spectroscopy is presently going through an explosive phase of development. This has been brought about largely on account of the advent of Fourier transform NMR spectrometers linked to powerful microcomputers which have opened up a whole new world for structural chemists and biochemists. This is exemplified by a host of

publications, especially on new pulse sequences, which continue to provide new exciting modifications for recording two-dimensional NMR. Moreover, NMR is no longer confined to structural chemists but has moved firmly into the area of medicine as a powerful nondestructive body scanning technique. With this background, I felt that there was need for a text which would provide a fairly comprehensive account of the important features of 1 H- and 13C-NMR spectroscopy in one book, as well as make available an up-to-date account of recent developments of new pulse sequences, with particular reference to 2D-NMR spectroscopy. Since this book is written for students of chemistry and biochemistry as well as for biology students who have chemistry as a subsidiary, it was decided to avoid a complex mathematical treatment and to present, as far as possible without oversimplification, a qualitative account of 1 H- and 13C-NMR spectroscopy as it is today. I hope that the book satisfactorily meets these objectives.

NMR in Chemistry Wiley

An understanding of spectroscopic techniques in the analysis of chemical structures is essential to all chemistry degree courses. This new addition to the Oxford Chemistry Primers series provides the essential material needed by undergraduates, in a compact form. It will be beneficial to postgraduates in organic chemistry as reference material in their daily research.

High-resolution NMR Techniques in Organic Chemistry John Wiley & Sons

Introduction to NMR Spectroscopy R. J. Abraham, School of Chemistry, University of Liverpool J. Fisher, Biological NMR Centre, University of Leicester P. Loftus, Stuart Pharmaceuticals, Delaware, USA This book is a new, extended edition of Proton and Carbon 13 NMR by R. J. Abraham and P. Loftus. The initial chapters cover the fundamentals of NMR spectroscopy commencing with an explanation of how the nuclear magnetic response occurs, followed by a detailed discussion of chemical shifts and coupling constants, parameters not discussed to any length in other textbooks aimed at a similar level of interest. Emphasis is given to the vectorial description of multipulse experiments, as this is probably the easiest way to grasp how different information may be gained simply by changing a pulse sequence. An understanding of multipulse NMR is a prerequisite for understanding 2D NMR. The section on 2D NMR begins with a discussion of the resolved experiment. This is a logical initial choice as the spectra produced by this experiment may be readily compared with 1D spectra. Following on from this both heteronuclear and homonuclear correlation spectroscopy are described and examples given. The final section of the book should be considered as an applications section. It is aimed at showing the reader that NMR is not just of use to the synthetic organic chemist but is also of use to biochemists for investigating the solution state structure

and function of proteins, enzymes, etc. The application of high resolution NMR to the solid state is also discussed, thereby indicating the developments which have taken place as far as spectrometer hardware is concerned.

Introduction to Functional Magnetic Resonance Imaging John Wiley & Sons Provides a theoretical introduction to graduate scientists and industrial researchers towards the understanding of the assignment of 1H NMR spectra Discusses, and includes on enclosed CD, one of the best, the fastest and most applicable pieces of NMR prediction software available Allows students of organic chemistry to solve problems on 1H NMR with access to over 500 assigned spectra

Biopolymer Science for Proteins and Peptides John Wiley & Sons

Nuclear magnetic resonance (NMR) spectroscopy is one of the most powerful and widely used techniques in chemical research for investigating structures and dynamics of molecules. Advanced methods can even be utilized for structure determinations of biopolymers, for example proteins or nucleic acids. NMR is also used in medicine for magnetic resonance imaging (MRI). The method is based on spectral lines of different atomic nuclei that are excited when a strong magnetic field and a radiofrequency transmitter are applied. The method is very sensitive to the features of molecular structure because also the neighboring atoms influence the signals from individual nuclei and this is important for determining the 3D-

structure of molecules. This new edition of the popular classic has a clear style and a highly practical, mostly non-mathematical approach. Many examples are taken from organic and organometallic chemistry, making this book an invaluable guide to undergraduate and graduate students of organic chemistry, biochemistry, spectroscopy or physical chemistry, and to researchers using this well-established and extremely important technique. Problems and solutions are included.

Basic 1H- and 13C-NMR Spectroscopy

Lulu.com

To date nitrogen NMR has been discussed in research papers and review articles throughout the scientific literature. It has been our aim in preparing this book to provide a comprehen sive account of the widely spread applications of nitrogen NMR. The relevant literature has been surveyed from the beginnings of NMR until early 1972. The steady annual growth in the number of references cited since 1965 is ample evidence of the ever increasing importance of the subject. Sufficient theoretical and experimental background is given for an understanding of the applications dealt with in later chapters. The basic principles of NMR are developed with a theoretical approach to chemical shifts and spin-spin coupling constants, particular emphasis being given to nitrogen nuclei. Following this the experimental aspects of nitrogen NMR are adequately described. Special

emphasis is given to the observable effects of the nuclear quadrupole moment of the 14 N nucleus. It is appro priate that this topic be dealt with in depth since quadrupolar interactions frequently dominate the information available from a study of the 14 N nucleus and other nuclei spin coupled to it. The applications of nitrogen chemical shift data to organic and inorganic molecules are covered in two extensive chapters which include the effects of paramagnetism on nitrogen NMR.
Spin Dynamics Springer Science & Business Media
Chiral Analysis covers an important area of analytical chemistry of relevance to a wide variety of scientific professionals. The target audience is scientific professionals with an undergraduate background in chemistry or a related discipline, specifically organic chemists, researchers in drug discovery, pharmaceutical researchers involved with process analysis or combinatorial libraries, and graduate students in chemistry. Chapters have been written with the nonspecialist in mind so as to be self-contained.* Broad coverage - spectroscopic and separation methods covered in a single volume* Up-to-date and detailed review of the various techniques available and/or under development in this field* Contributions from leading experts in the field
Profiles of Drug Substances, Excipients, and Related Methodology John Wiley & Sons
NMR Spectroscopy Explained : Simplified Theory, Applications and Examples for

Organic Chemistry and Structural Biology provides a fresh, practical guide to NMR for both students and practitioners, in a clearly written and non-mathematical format. It gives the reader an intermediate level theoretical basis for understanding laboratory applications, developing concepts gradually within the context of examples and useful experiments. Introduces students to modern NMR as applied to analysis of organic compounds. Presents material in a clear, conversational style that is appealing to students. Contains comprehensive coverage of how NMR experiments actually work. Combines basic ideas with practical implementation of the spectrometer. Provides an intermediate level theoretical basis for understanding laboratory experiments. Develops concepts gradually within the context of examples and useful experiments. Introduces the product operator formalism after introducing the simpler (but limited) vector model.

Nitrogen NMR Oxford University Press Applications of NMR Spectroscopy is a book series devoted to publishing the latest advances in the applications of nuclear magnetic resonance (NMR) spectroscopy in various fields of organic chemistry, biochemistry, health and agriculture. The fifth volume of the series features several reviews focusing on NMR spectroscopic techniques for identifying natural and synthetic compounds (polymer and peptide characterization, GABA in tinnitus affected mice), medical diagnosis and

therapy (gliomas) and food analysis. The spectroscopic methods highlighted in this volume include high resolution proton magnetic resonance spectroscopy and solid state NMR.
Proton and Carbon NMR Spectra of Polymers John Wiley & Sons
Nuclear Magnetic Resonance is a powerful tool, especially for the identification of 1 13 hitherto unknown organic compounds. H- and C-NMR spectroscopy is known and applied by virtually every synthetically working Organic Chemist. Con- quently, the factors governing the differences in chemical shift values, based on chemical environment, bonding, temperature, solvent, pH, etc. , are well understood, and specialty methods developed for almost every conceivable structural challenge. Proton and carbon NMR spectroscopy is part of most bachelors degree courses, with advanced methods integrated into masters degree and other graduate courses. In view of this universal knowledge about proton and carbon NMR spectr- copy within the chemical community, it is remarkable that heteronuclear NMR is still looked upon as something of a curiosity. Admittedly, most organic compounds contain only nitrogen, oxygen, and sulfur atoms, as well as the obligatory hydrogen and carbon atoms, elements that have an unfavourable isotope distribution when it comes to NMR spectroscopy. Each of these three elements has a dominant isotope: 14 16 32 16 32 N (99. 63% natural abundance), O (99. 76%), and S (95.

02%), with O, S, and 34 14 S (4. 21%) NMR silent. N has a nuclear moment I = 1 and a sizeable quadrupolar moment that makes the NMR signals usually very broad and dif cult to analyse.

Interpretation of NMR Spectra Walter de Gruyter GmbH & Co KG

This book presents a critical assessment of progress on the use of nuclear magnetic resonance spectroscopy to determine the structure of proteins, including brief reviews of the history of the field along with coverage of current clinical and in vivo applications. The book, in honor of Oleg Jardetsky, one of the pioneers of the field, is edited by two of the most highly respected investigators using NMR, and features contributions by most of the leading workers in the field. It will be valued as a landmark publication that presents the state-of-the-art perspectives regarding one of today's most important technologies.

Protein NMR Spectroscopy Springer Science & Business Media

This book describes the advanced developments in methodology and applications of NMR spectroscopy to life science and materials science. Experts who are leaders in the development of new methods and applications of life and material sciences have contributed an exciting range of topics that cover recent advances in structural determination of biological and material molecules, dynamic aspects of biological and material molecules, and development of novel NMR techniques, including resolution and sensitivity

enhancement. First, this book particularly emphasizes the experimental details for new researchers to use NMR spectroscopy and pick up the potentials of NMR spectroscopy. Second, the book is designed for those who are involved in either developing the technique or expanding the NMR application fields by applying them to specific samples. Third, the Nuclear Magnetic Resonance Society of Japan has organized this book not only for NMR members of Japan but also for readers worldwide who are interested in using NMR spectroscopy extensively.

Problems and Solution in Proton NMR Spectroscopy Free Press

With the development in recent years of NMR spectrometers capable of recording with a minimum of effort data that are both accurate and reproducible, a need has arisen for spectra catalogs and data books to aid the researcher. The ability to correlate a spectrum to a precalibrated chart accurately (to within 0. 02 ppm) has made chemical shift, along with the character of the spectral lines produced, an increasingly important tool in configurational analysis-a tool which this book is designed to complement. It is known that the chemical shift of a proton can be influenced by atoms as much as five or six carbons away, a fact of great importance to compound identification. The entries in this book, arranged according to proton environment, enable the researcher with a hypo thetical structure already proposed for his unknown quickly to locate examples of

compounds having similar structures. An index of molecular formulas and a shift index, which should prove useful in hypothesizing alternate structures for the unknown and in checking out the hypotheses, have also been provided. The data collected represent some 4800 shifts from the spectra of about 1200 compounds that appear in the catalogs of Varian Associates, Sadtler Research Laboratories, and the American Petroleum Institute, whose cooperation is gratefully acknowledged. The alphanumerical code that is the basis of our presentation, and the explanation of its use, are borrowed intact from the NMR Spectra Catalog of Varian Associates, for whose permission to use this material we are especially grateful.

NMR Spectroscopy of Polymers John Wiley & Sons

Combines clear and concise discussions of key NMR concepts with succinct and illustrative examples Designed to cover a full course in Nuclear Magnetic Resonance (NMR) Spectroscopy, this text offers complete coverage of classic (one-dimensional) NMR as well as up-to-date coverage of two-dimensional NMR and other modern methods. It contains practical advice, theory, illustrated applications, and classroom-tested problems; looks at such important ideas as relaxation, NOEs, phase cycling, and processing parameters; and provides brief, yet fully comprehensible, examples. It also uniquely lists all of the general parameters for many experiments including mixing times, number of scans, relaxation times, and

more. Nuclear Magnetic Resonance Spectroscopy: An Introduction to Principles, Applications, and Experimental Methods, 2nd Edition begins by introducing readers to NMR spectroscopy - an analytical technique used in modern chemistry, biochemistry, and biology that allows identification and characterization of organic, and some inorganic, compounds. It offers chapters covering: Experimental Methods; The Chemical Shift; The Coupling Constant; Further Topics in One-Dimensional NMR Spectroscopy; Two-Dimensional NMR Spectroscopy; Advanced Experimental Methods; and Structural Elucidation. Features classical analysis of chemical shifts and coupling constants for both protons and other nuclei, as well as modern multi-pulse and multi-dimensional methods Contains experimental procedures and practical advice relative to the execution of NMR experiments Includes a chapter-long, worked-out problem that illustrates the application of nearly all current methods Offers appendices containing the theoretical basis of NMR, including the most modern approach that uses product operators and coherence-level diagrams By offering a balance between volumes aimed at NMR specialists and the structure-determination-only books that focus on synthetic organic chemists, Nuclear Magnetic Resonance Spectroscopy: An Introduction to Principles, Applications, and Experimental Methods, 2nd Edition is an excellent text for students and post-graduate students working in analytical

and bio-sciences, as well as scientists who use NMR spectroscopy as a primary tool in their work.

Biological NMR Spectroscopy Springer Science & Business Media

Clear, accessible coverage of modern NMR spectroscopy-for students and professionals in many fields of science Nuclear magnetic resonance (NMR) spectroscopy has made quantum leaps in the last decade, becoming a staple tool in such divergent fields as chemistry, physics, materials science, biology, and medicine. That is why it is essential that scientists working in these areas be fully conversant with current NMR theory and practice. This down-to-basics text offers a comprehensive, up-to-date treatment of the fundamentals of NMR spectroscopy. Using a straightforward approach that develops all concepts from a rudimentary level without using heavy mathematics, it gives readers the knowledge they need to solve any molecular structure problem from a complete set of NMR data. Topics are illustrated throughout with hundreds of figures and actual spectra. Chapter-end summaries and review problems with answers are included to help reinforce and test understanding of key material. From NMR studies of biologically important molecules to magnetic resonance imaging, this book serves as an excellent all-around primer on NMR spectroscopic analysis.

A Complete Introduction to Modern NMR Spectroscopy Academic Press

Protein NMR Spectroscopy, Second Edition combines a comprehensive

theoretical treatment of NMR spectroscopy with an extensive exposition of the experimental techniques applicable to proteins and other biological macromolecules in solution. Beginning with simple theoretical models and experimental techniques, the book develops the complete repertoire of theoretical principles and experimental techniques necessary for understanding and implementing the most sophisticated NMR experiments. Important new techniques and applications of NMR spectroscopy have emerged since the first edition of this extremely successful book was published in 1996. This updated version includes new sections describing measurement and use of residual dipolar coupling constants for structure determination, TROSY and deuterium labeling for application to large macromolecules, and experimental techniques for characterizing conformational dynamics. In addition, the treatments of instrumentation and signal acquisition, field gradients, multidimensional spectroscopy, and structure calculation are updated and enhanced. The book is written as a graduate-level textbook and will be of interest to biochemists, chemists, biophysicists, and structural biologists who utilize NMR spectroscopy or wish to understand the latest developments in this field. - Provides an understanding of the theoretical principles important for biological NMR spectroscopy - Demonstrates how to implement, optimize and troubleshoot modern multi-

dimensional NMR experiments - Allows for the capability of designing effective experimental protocols for investigations of protein structures and dynamics - Includes a comprehensive set of example NMR spectra of ubiquitin provides a reference for validation of experimental methods

Understanding NMR Spectroscopy John Wiley & Sons

A visual guide for the interpretation of complex 1H-NMR spectra with a concise and illustrative practice problems section. This book is an easy-to-grasp source for (organic) chemists and students that want to understand and practice NMR spectroscopy.

Applied NMR Spectroscopy for Chemists and Life Scientists John Wiley & Sons

This book contains Basic question and exercises on Proton NMR which is very useful for both Graduate and Postgraduate student to learn how to interpret NMR spectra.

Calculation of NMR and EPR Parameters Elsevier

NMR Spectroscopy of the Non-Metallic Elements Stefan Berger Philipps-Universität, Marburg, Germany Siegmar Braun Technische Hochschule Darmstadt, Germany Hans-Otto Kalinowski Justus-Liebig-Universität, Gießen, Germany In recent years, the technique of Nuclear Magnetic Resonance (NMR) Spectroscopy has rapidly gained in importance outside its traditional areas of proton NMR and carbon-13 NMR. In particular, it has become much more applicable to compounds containing elements such as

phosphorus, nitrogen and fluorine. NMR Spectroscopy of the Non-Metallic Elements gathers together a wealth of NMR data for the most important non-metallic elements, namely nitrogen, oxygen, fluorine, phosphorus, sulphur and xenon. For each element, the data for the simpler compounds and their derivatives (both organic and inorganic) are gathered together in as complete a form as possible, and the regularities that emerge are discussed in detail in relation to structural variations. This allows the reader to interpret the structure of more complex structures. The chapters containing the NMR data for the elements are preceded by a practical introduction to the basic theory and experimental techniques of the NMR parameters, especially the chemical shift and indirect spin-spin coupling. This material will help the reader both in finding practical solutions to problems of structure determination, and in critically evaluating the spectra obtained. NMR Spectroscopy of the Non-Metallic Elements is an invaluable reference source for all laboratories where NMR is used. It will also be widely used by organic and inorganic chemists, especially those working on nitrogen, fluorine and phosphorus compounds.