Understanding Nmr Spectroscopy

NMR Spectroscopy Techniques, Second Edition,
Solid State NMR Spectroscopy
Principles of NMR Spectroscopy
Proton and Carbon-13 Nmr Spectroscopy
A Practical Guide to Understanding the NMR of Polymers
Methodology and Application to Life Science and Materials Science
Modelling 1H NMR Spectra of Organic Compounds
Organic Structures from 2D NMR Spectra
Structure of High-Resolution NMR Spectra
Basic Principles, Concepts and Applications in Chemistry
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NMR Spectroscopy Techniques, Second Edition, Springer Science & Business Media
NMR Spectroscopy using Liquid Crystal Solvents covers the importance of using a liquid crystal solvent in NMR to derive nuclear dipolar spin-spin coupling constants. This book is composed of ten chapters, and begins with a brief description of the features and benefits of liquid crystal in NMR spectroscopic analysis. The succeeding chapters deal with the mode of operation of nuclear spin Hamiltonian for partially oriented molecules and the analysis of NMR spectra of partially oriented molecules, as well as the determination of rigid molecule structure. These topics are followed by discussions on internal motion studies, NMR spectra from quadpolar nuclei, and the anisotropy in nuclear spin-spin coupling. The final chapters review the theoretical and experimental studies on the anisotropy in chemical shifts, nematic rotation, and the nuclear magnetic double resonance. This book will prove useful to analytical chemists.
Solid State NMR Spectroscopy John Wiley & Sons
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.
Principles of NMR Spectroscopy IOS Press
NMR Spectroscopy in Liquids and Solids provides an introduction of the general concepts behind Nuclear Magnetic Resonance (NMR) and its applications, including how to perform adequate NMR experiments and interpret data collected in liquids and solids to characterize molecule systems in terms of their structure and dynamics. The book is composed of ten chapters. The first three chapters consider the theoretical basis of NMR spectroscopy, the theory of NMR relaxation, and the practice of relaxation measurements. The middle chapters discuss the general aspects of molecular dynamics and their relationships to NMR, NMR spectroscopy and relaxation studies in solutions, and special issues related to NMR in solutions. The remaining chapters introduce general principles and strategies involved in solid-state NMR studies, provide examples of applications of relaxation for the determination of molecular dynamics in diamagnetic solids, and discuss special

issues related to solid state NMR—including NMR relaxation in paramagnetic solids. All chapters are accompanied by references and recommended literature for further reading. Many practical examples of multinuclear NMR and relaxation experiments and their interpretations are also presented. The book is ideal for scientists new to NMR, students, and investigators working in the areas of chemistry, biochemistry, biology, pharmaceutical sciences, or materials science.

Proton and Carbon-13 Nmr Spectroscopy Walter de Gruyter GmbH & Co KG

The derivation of structural information from spectroscopic data is now an integral part of organic chemistry courses at all Universities. Over recent years, a number of powerful two-dimensional NMR techniques (e.g. HSQC, HMBC, TOCSY, COSY and NOESY) have been developed and these have vastly expanded the amount of structural information that can be obtained by NMR spectroscopy. Improvements in NMR instrumentation now mean that 2D NMR spectra are routinely (and sometimes automatically) acquired during the identification and characterisation of organic compounds. Organic Structures from 2D NMR Spectra is a carefully chosen set of more than 60 structural problems employing 2D-NMR spectroscopy. The problems are graded to develop and consolidate a student's understanding of 2D NMR spectroscopy. There are many easy problems at the beginning of the collection, to build confidence and demonstrate the basic principles from which structural information can be extracted using 2D NMR. The accompanying text is very descriptive and focussed on explaining the underlying theory at the most appropriate level to sufficiently tackle the problems. Organic Structures from 2D NMR Spectra Is a graded series of about 60 problems in 2D NMR spectroscopy that assumes a basic knowledge of organic chemistry and a basic knowledge of one-dimensional NMR spectroscopy Incorporates the basic theory behind 2D NMR and those common 2D NMR experiments that have proved most useful in solving structural problems in organic chemistry Focuses on the most common 2D NMR techniques – including COSY, NOESY, HMBC, TOCSY, CH-Correlation and multiplicity-edited C-H Correlation. Incorporates several examples containing the heteronuclei 31P, 15N and 19F Organic Structures from 2D NMR Spectra is a logical follow-on from the highly successful "Organic Structures from Spectra" which is now in its fifth edition. The book will be invaluable for students of Chemistry, Pharmacy, Biochemistry and those taking courses in Organic Chemistry. Also available: Instructors Guide and Solutions Manual to Organic Structures from 2D NMR Spectra

A Practical Guide to Understanding the NMR of Polymers Springer

The renowned Oxford Chemistry Primers series, which provides focused introductions to a range of important topics in chemistry, has been refreshed and updated to suit the needs of today's students, lecturers, and postgraduate researchers. The rigorous, yet accessible, treatment of each subject area is ideal for those wanting a primer in a given topic to prepare them for more advanced study or research. NMR: The Toolkit describessuccinctly the range of NMR techniques commonly used in modern research to probe the structures and properties of molecules in

liquids. Emphasis is placed throughout on how these experiments actually work, givinga unique perspective on this powerful experimental tool.
Methodology and Application to Life Science and Materials Science 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
Modelling 1H NMR Spectra of Organic Compounds John Wiley & Sons
During the last two decades, the use of NMR spectroscopy for the characterization and analysis of food materials has flourished, and this trend continues to increase today. Currently, there exists no book that fulfils specifically the needs of food scientists that are interested in adding or expanding the use of NMR spectroscopy in their arsenal of food analysis techniques. Current books and monographs are rather addressed to experienced researchers in food analysis providing new information in the field. This book, written by acknowledged experts in the field, fills the gap by offering a day to day NMR guide for the food scientist, affording not only the basic theoretical aspects of NMR spectroscopy, but also practical information on sample preparation, experimental conditions and data analysis. Current developments in the field covered in this book are the availability of solid state NMR experiments such as CP/MAS and more importantly HR-MAS NMR for the analysis of semisolid foods, and the increasing use of chemometrics to analyze NMR data in food metabonomics. Moreover, this book contains an up to date discussion of MRI in food analysis including topics such as food processing and natural changes in food such as ripening. The book is a compact and complete source of information for food scientists who wish to apply methodologies based on NMR spectroscopy in food analysis. It contains information so far scattered in the primary literature, in NMR treatises and food analysis books, in a concise format that makes it appealing to food scientists who have no or minimal experience in magnetic resonance techniques. The inclusion of practical information about NMR instrumentation, experiment setup, acquisition and spectral analysis for the study of different food categories make this book a hands-on manual for food scientists wishing to implement novel NMR spectroscopy-based analytical techniques in their field.
Organic Structures from 2D NMR Spectra John Wiley & Sons
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

Structure of High-Resolution NMR Spectra Academic Press

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.

Basic Principles, Concepts and Applications in Chemistry John Wiley & Sons

Through numerous examples, the principles of the relationship between chemical structure and the NMR spectrum are developed in a logical, step-by-step fashion Includes examples and exercises based on real NMR data including full 600 MHz one- and two-dimensional datasets of sugars, peptides, steroids and natural products Includes detailed solutions and explanations in the text for the numerous examples and problems and also provides large, very detailed and annotated sets of NMR data for use in understanding the material Describes both simple aspects of solution-state

NMR of small molecules as well as more complex topics not usually covered in NMR books such as complex splitting patterns, weak long-range couplings, spreadsheet analysis of strong coupling patterns and resonance structure analysis for prediction of chemical shifts Advanced topics include all of the common two-dimensional experiments (COSY, ROESY, NOESY, TOCSY, HSQC, HMBC) covered strictly from the point of view of data interpretation, along with tips for parameter settings

NMR Spectroscopy in Food Analysis Elsevier

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful and theoretically complex analytical tool. Basic 1H- and 13C-NMR Spectroscopy provides an introduction to the principles and applications of NMR spectroscopy. Whilst looking at the problems students encounter when using NMR spectroscopy, the author avoids the complicated mathematics that are applied within the field. Providing a rational description of the NMR phenomenon, this book is easy to read and is suitable for the undergraduate and graduate student in chemistry. Describes the fundamental principles of the pulse NMR experiment and 2D NMR spectra Easy to read and written with the undergraduate and graduate chemistry student in mind Provides a rational description of NMR spectroscopy without complicated mathematics

NMR Spectroscopy in Organic Chemistry John Wiley & Sons

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.

Volume 45 Springer Science & Business Media

NMR spectroscopy has proven to be a powerful technique to study the structure and dynamics of biological macromolecules. Fundamentals of Protein NMR Spectroscopy is a comprehensive textbook that guides the reader from a basic understanding of the phenomenological properties of magnetic resonance to the application and interpretation of modern multi-dimensional NMR experiments on 15N/13C-labeled proteins. Beginning with elementary quantum mechanics, a set of practical rules is presented and used to describe many commonly employed multi-dimensional, multi-nuclear NMR pulse sequences. A modular analysis of NMR pulse sequence building blocks also provides a basis for understanding and developing novel pulse programs. This text not only covers topics from chemical shift assignment to protein structure refinement, as well as the analysis of protein dynamics and chemical kinetics, but also provides a practical guide to many aspects of modern spectrometer hardware, sample preparation, experimental set-up, and data processing. End of chapter exercises are included to emphasize important concepts. Fundamentals of Protein NMR Spectroscopy not only offer students a systematic, in-depth, understanding of

modern NMR spectroscopy and its application to biomolecular systems, but will also be a useful reference for the experienced investigator.

NMR Spectroscopy Explained John Wiley & Sons

Nuclear Magnetic Resonance (NMR) spectroscopy is the most powerful technique for characterization of biomolecular structures at atomic resolution in the solution state. This timely book, entitled "Biomolecular NMR Spectroscopy," focuses on the latest state-of-the-art NMR techniques for characterization of biological macromolecules in the solid and solution state. The editors, Dr. Andrew Dingley (University of Auckland, New Zealand) and Dr. Steven Pascal (Massey University, New Zealand) have organized the book into four sections, covering the following topics: sample preparation, structure and dynamics of proteins, structure and dynamics of nucleic acids and protein-nucleic acid complexes, and rapid and hybrid techniques--

Experimental Approaches of NMR Spectroscopy Elsevier

In recent years high-resolution nuclear magnetic resonance spec troscopy has found very wide application in organie chemistry in structural and physicochemical investigations and. also in the study of the characteristics of organic compounds which are re lated to the distribution of the electron cloud in the molecules. The vigorous development of this method, which may really be re garded as an independent branch of science, is the result of ex tensive progress in NMR technology, the refinement of its theory, and the accumulation of large amounts of experimental material, which has been correlated by empiricallaws and principles. The literature directly concerned with the NMR method and its applica tion has now grown to such an extent that a complete review of it is practically impossible. Therefore the authors have limited themselves to an examination of only the most important, funda mental, and general investigations. The book consists of six chapters. In the first chapter we have attempted to present the fundamentals of the NMR method in such a way that the reader with little knowledge of the subject will be able to use the method in practical work for investigating simple compounds and solving simple problems. The three subsequent chapters give a deeper analysis of the method, while the last two chapters and the appendix illustrate the various applications of NMR spectroscopy in organic chemistry.

NMR Spectroscopy Elsevier

Introduction to Solid State NMR Spectroscopy is written for undergraduate and graduate students of chemistry, either taking a course in advanced or solid-state nuclear magnetic resonance spectroscopy or undertaking research projects where solid-state NMR is likely to be a major investigative technique. It will also serve as a practical introduction in industry, where the techniques can provide new or complementary information to supplement other investigative techniques. By covering solid-state NMR spectroscopy in a clear, straightforward and approachable way with detailed descriptions of the major solid-state NMR experiments focussing on what the experiments do and what they tell the researcher, this book will serve as an ideal introduction to the subject. These descriptions are backed up by separate mathematical explanations for those who wish to gain a more sophisticated

quantitative understanding of the phenomena. With additional coverage of the practical implementation of solid-state NMR experiments integrated into the discussion, this book will be essential reading for all those using, or about to use, solid-state NMR spectroscopy. Dr Melinda Duer is a senior lecturer in the Department of Chemistry at the University of Cambridge, Cambridge, UK.
NMR Spectroscopy Using Liquid Crystal Solvents Springer Science & Business Media
Presents basic concepts, experimental methodology and data acquisition, and processing standards of in vivo NMR spectroscopy This book covers, in detail, the technical and biophysical aspects of in vivo NMR techniques and includes novel developments in the field such as hyperpolarized NMR, dynamic 13C NMR, automated shimming, and parallel acquisitions. Most of the techniques are described from an educational point of view, yet it still retains the practical aspects appreciated by experimental NMR spectroscopists. In addition, each chapter concludes with a number of exercises designed to review, and often extend, the presented NMR principles and techniques. The third edition of In Vivo NMR Spectroscopy: Principles and Techniques has been updated to include experimental detail on the developing area of hyperpolarization; a description of the semi-LASER sequence, which is now a method of choice; updated chemical shift data, including the addition of 31P data; a troubleshooting section on common problems related to shimming, water suppression, and quantification; recent developments in data acquisition and processing standards; and MatLab scripts on the accompanying website for helping readers calculate radiofrequency pulses. Provide an educational explanation and overview of in vivo NMR, while maintaining the practical aspects appreciated by experimental NMR spectroscopists Features more experimental methodology than the previous edition End-of-chapter exercises that help drive home the principles and techniques and offer a more in-depth exploration of quantitative MR equations Designed to be used in conjunction with a teaching course on the subject In Vivo NMR Spectroscopy: Principles and Techniques, 3rd Edition is aimed at all those involved in fundamental and/or diagnostic in vivo NMR, ranging from people working in dedicated in vivo NMR institutes, to radiologists in hospitals, researchers in high-resolution NMR and MRI, and in areas such as neurology, physiology, chemistry, and medical biology.
In Vivo NMR Spectroscopy John Wiley & Sons
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

High-resolution NMR Techniques in Organic Chemistry Oxford University Press

Since the first successful NMR experiments in 1946 it was well appreciated that dynamic processes play an important role in the NMR spectroscopy of bulk matter [1]. Early theories on the dependence of the relaxation parameters Tl and T2 on the motions of nuclear spins were successful in explaining the dipolar broadening of the NMR signal in solids and the motional narrowing in liquids [2]. With the discovery of chemical shifts and spin-spin couplings another type of dynamical process affect ing the NMR line shape became apparent, the chemical exchange. As a consequence, dynamical NMR studies split into two groups differing not only in the dynamical topics but also in the method of investigation: physical studies of the motion of spins in liquids and solids by measurement of the relaxation times of single resonances and, on the other hand, chemical studies based on band shape analysis of NMR spectra recorded under steady state conditions. The two fields of research lost some of their basic differences with the development of the Fourier transform NMR method [3], which allows the measurement of relaxation times of different resonances at the same time, i. e. the study of differential motional behavior of different parts of mole cules, thus providing a new tool in conformational analyses. For example, informa tion can be obtained by this method on the relative importance of overall motions and internal motions [4].

Annual Reports on NMR Spectroscopy John Wiley & Sons

Understanding NMR SpectroscopyJohn Wiley & Sons

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