

# Understanding NMR Spectroscopy

SECOND EDITION

**James Keeler**, *Department of Chemistry, University of Cambridge, UK*

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 step-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  $AX_n$  and  $AX_nX_m$  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*



**Dr James Keeler** is a Senior Lecturer in Chemistry at the University of Cambridge, and a Fellow of Selwyn College. In addition to being actively involved in the development of new NMR techniques, he is also responsible for the undergraduate chemistry course, and is Editor-in-Chief of *Magnetic Resonance in Chemistry*. Dr Keeler is well-known for his clear and accessible exposition of NMR spectroscopy.

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# Understanding Nmr Spectroscopy

**Neil E. Jacobsen**



## Understanding Nmr Spectroscopy:

**Understanding NMR Spectroscopy** James Keeler, 2011-09-19 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 *Understanding NMR Spectroscopy* Ray Freeman, James Keeler, 1990 *Understanding NMR Spectroscopy* James Keeler, 2005-12-06 *Understanding NMR Spectroscopy* James Keeler Department of Chemistry University of Cambridge UK This text discusses the high resolution NMR of liquid samples and concentrates exclusively on spin half nuclei mainly 1H and 13C It is aimed at people who are familiar with the use of routine NMR for structure determination and who wish to deepen their understanding of just exactly how NMR experiments work It demonstrates that in NMR it is possible quite literally on the back of an envelope to make exact predictions of the outcome of quite sophisticated experiments The experiments chosen are likely to be encountered in the routine NMR of small to medium sized molecules but are also applicable to the study of large biomolecules such as proteins and nucleic acids The book starts off at a gentle pace working through some more or less familiar ideas and then elaborating these as the book progresses Each chapter ends with exercises which are designed to assist in the understanding of the ideas presented and to grasp the underlying ideas **NMR Spectroscopy Explained** Neil E. Jacobsen, 2007-08-27 *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

Introduction to NMR Spectroscopy Raymond John Abraham, J. Fisher, P. Loftus, 1988-11-24 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 **Protein NMR Spectroscopy** John Cavanagh, Nicholas J. Skelton, Wayne J. Fairbrother, Mark Rance, Arthur G. Palmer III, 2010-07-21 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

**Optimising NMR Spectroscopy Through Method and Software Development** Jonathan Yong,2024-01-09 This book provides a comprehensive overview of Nuclear Magnetic Resonance NMR theory its applications and advanced techniques to improve the quality and speed of NMR data acquisition In this book the author expands his outstanding Ph D thesis and provides a valuable resource for researchers professionals and students in the field of NMR spectroscopy The book covers quantum mechanics basics and topics like density operators pulse sequences 1D pulse acquisition INEPT Insensitive nuclei enhancement by polarization transfer product operators and 2D NMR principles It also explores innovative experiments like States HSQC Heteronuclear Single Quantum Coherence and echo antiecho HSQC with gradients In the subsequent chapters the author discusses Pure Shift NMR including PSYCHE Pure Shift Yielded by Chirp Excitation and its optimizations such as waveform parameterization and time reversal methods The Discrete PSYCHE approach and Ultrafast PSYCHE iDOSY Diffusion ordered spectroscopy are also highlighted This book presents the POISE Parameter Optimisation by Iterative Spectral Evaluation software for real time NMR experiment optimization including pulse width calibration and Ernst angle optimization and demonstrates applications across various NMR experiments Lastly the book examines accelerated 2D NMR data collection and the NOAH NMR by Ordered Acquisition using  $^1\text{H}$  detection supersequences emphasizing automated pulse program creation using GENESIS GENERation of Supersequences In Silico Covered NMR experiments include  $^{13}\text{C}$  sensitivity enhanced HSQC  $^{15}\text{N}$  HMQC Heteronuclear Multiple Quantum Coherence dual HSQC HSQC TOCSY Total Correlation Spectroscopy HMBG Heteronuclear Multiple Bond Correlation and ADEQUATE Adequate Sensitivity Double Quantum Spectroscopy

**Protein NMR Spectroscopy** Lu-Yun Lian,Gordon Roberts,2011-08-08 Nuclear Magnetic Resonance NMR spectroscopy a physical phenomenon based upon the magnetic properties of certain atomic nuclei has found a wide range of applications in life sciences over recent decades This up to date volume covers NMR techniques and their application to proteins with a focus on practical details Providing newcomers to NMR with practical guidance to carry out successful experiments with proteins and analyze the resulting spectra those familiar with the chemical applications of NMR will also find it useful in understanding the special requirements of protein NMR

*Fundamentals of Protein NMR Spectroscopy* Gordon S. Rule,T. Kevin Hitchens,2005-10-28 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  $^{15}\text{N}$   $^{13}\text{C}$  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

**Spin Dynamics** Malcolm H. Levitt, 2001-12-05 NMR spectroscopy is one of the most important and widely used techniques for the identification of compounds Based on an established course this core text offers a truly modern and updated approach Provides a comprehensive introduction to the subject Includes a multi disciplinary approach concentrating on basic principles and concepts Contains chapters of worked examples and problems to encourage a fuller understanding of topics Offers a pedagogical approach starting with quarks and nucleons and moving on to cover NMR imaging COSY Correlated Spectroscopy and NOESY Nuclear Overhauser Effect Spectroscopy As a core subject in many science disciplines this text will appeal to a wide range of students as well as practising scientists and technicians Assuming only a basic knowledge of complex numbers and matrices it carefully and lucidly aids readers to fully understand this challenging subject

*NMR Data Interpretation Explained* Neil E. Jacobsen, 2016-10-21 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

*50 and More Essential NMR Experiments* Matthias Findeisen, Stefan Berger, 2013-07-30 This book is the perfect link for learning how to perform the experiments after only having studied theory In eight chapters more than 50 essential NMR experiments are described in detail Special focus is put on the organic set of NMR spectra  $^1\text{H}$   $^{13}\text{C}$  APT COSY NOESY HSQC and HMBC Different chapters deal with advanced organic NMR selective

methods heteronuclear NMR relaxation and diffusion measurements organic applications and maintenance Every experiment has a section providing the reader with the purpose and scope of the specific experiment Every experiment is concluded with the spectrum as it is obtained under the conditions described Questions and comments enable the reader to check their understanding The authors are very experienced and the whole book is in full color which enhances the reading experience and makes the spectra and other figures easier to understand This book is strongly recommended for all students and researchers who are involved in the structural elucidation of chemical compounds both in practical education and in pursuing research in particular if they handle an NMR spectrometer NMR - From Spectra to Structures Terence N.

Mitchell, Burkhard Costisella, 2007-08-14 Nuclear magnetic resonance spectroscopy is one of the most powerful analytical methods This practice oriented textbook aims at teaching how NMR experiments should be used to make structural assignments The book is intended as a practical guide for students and laboratory personnel so that the emphasis is on practical rather than on theoretical aspects which are treated only to the extent necessary to understand the experiments and to interpret the results The second edition has been expanded to include several other heteronuclei  $^{15}\text{N}$   $^{19}\text{F}$   $^{29}\text{Si}$   $^{77}\text{Se}$   $^{113}\text{Cd}$   $^{117}\text{Sn}$   $^{119}\text{Sn}$   $^{195}\text{Pt}$   $^{207}\text{Pb}$  and a new chapter on solid state NMR The problems section has been enlarged and now includes 50 problems These are of different degrees of complexity and in all cases include two dimensional 2D methods as well as standard proton and carbon 1D spectra **High Resolution NMR Spectroscopy: Understanding Molecules and their Electronic Structures**, 2013-06-08

The progress in nuclear magnetic resonance NMR spectroscopy that took place during the last several decades is observed in both experimental capabilities and theoretical approaches to study the spectral parameters The scope of NMR spectroscopy for studying a large series of molecular problems has notably broadened However at the same time it requires specialists to fully use its potentialities This is a notorious problem and it is reflected in the current literature where this spectroscopy is typically only used in a routine way Also it is seldom used in several disciplines in which it could be a powerful tool to study many problems The main aim of this book is to try to help reverse these trends This book is divided in three parts dealing with 1 high resolution NMR parameters 2 methods for understanding high resolution NMR parameters and 3 some experimental aspects of high resolution NMR parameters for studying molecular structures Each part is divided into chapters written by different specialists who use different methodologies in their work In turn each chapter is divided into sections Some features of the different sections are highlighted it is expected that part of the readership will be interested only in the basic aspects of some chapters while other readers will be interested in deepening their understanding of the subject dealt with in them Shows how NMR parameters are useful for structure assignment as well as to obtain insight on electronic structures Emphasis on conceptual aspects Contributions by specialists who use the discussed methodologies in their everyday work **NMR Spectroscopy** Christian Schorn, Brian F. Taylor, 2004 This volume enables the newcomer to become familiar with the basic data acquisition procedures modular pulse sequence

units and complete sequences in NMR spectroscopy      **NMR Spectroscopy** Myrna J. Simpson, Andre J. Simpson, 2014-06-12

The challenges faced by environmental scientists today are vast complex and multi faceted For instance predicting the fate of an environmental pollutant or understanding ecosystem responses to climate change necessitate a firm understanding of molecular structure and dynamics of environmental media as well as the components that exist and interact within this media Furthermore linking information obtained at the molecular scale to ecosystem level processes is a major pursuit of modern environmental research As such NMR spectroscopy and its scalability from the molecular scale to the macroscopic scale is facilitating rapid growth in environmental science In addition the versatility of NMR spectroscopy has resulted in the development and implementation of different types of NMR techniques to examine the structure of various types of environmental samples living and non living as well as the study of critical environmental processes This comprehensive handbook is a collection of chapters that span from methods to how NMR is used in environmental research to gain insight into various ecosystem properties It is organized into three parts Part A focuses on methods used in environmental NMR which span from solution state to magnetic resonance imaging Part B emphasizes how NMR spectroscopy plays an essential role in understanding various types of environmental components and related processes including different forms of organic matter found in soil water and air as well as how NMR is used to probe the fate of water organic pollutants and metals in the environment Part C focuses on the growing field of environmental metabolomics which uses NMR as its main discovery platform This volume highlights the immense potential of NMR spectroscopy to expand our fundamental understanding of environmental processes and how it will continue to do so well into the future About eMagRes Handbooks eMagRes formerly the Encyclopedia of Magnetic Resonance publishes a wide range of online articles on all aspects of magnetic resonance in physics chemistry biology and medicine The existence of this large number of articles written by experts in various fields is enabling the publication of a series of eMagRes Handbooks on specific areas of NMR and MRI The chapters of each of these handbooks will comprise a carefully chosen selection of eMagRes articles In consultation with the eMagRes Editorial Board the eMagRes handbooks are coherently planned in advance by specially selected Editors and new articles are written to give appropriate complete coverage The handbooks are intended to be of value and interest to research students postdoctoral fellows and other researchers learning about the scientific area in question and undertaking relevant experiments whether in academia or industry Have the content of this handbook and the complete content of eMagRes at your fingertips Visit [www.wileyonlinelibrary.com/ref/eMagRes](http://www.wileyonlinelibrary.com/ref/eMagRes)

Two-dimensional NMR Spectroscopy William R. Croasmun, Robert M. K. Carlson, 1994      *Principles of NMR Spectroscopy* David Goldenberg, 2016-03-31 With nearly 400 original illustrations this NMR primer provides an introduction to solution NMR spectroscopy at a level appropriate for advanced undergraduates graduate students and working scientists with backgrounds in chemistry or biochemistry With nearly 400 original illustrations this NMR primer provides an introduction to solution NMR spectroscopy at a level appropriate for advanced



undergraduates graduate students and working scientists with backgrounds in chemistry or biochemistry It presents the underlying physics and mathematics in a way that is both accessible and sufficiently complete to allow a real understanding of modern multi dimensional experiments thereby giving readers the tools they need to move to more advanced textbooks and articles One special feature of this text is a thorough but accessible treatment of spin quantum mechanics including scalar coupled spins A novel style of vector diagram is used to represent the quantum correlations between coupled spins and the manipulation of these correlations by pulses and time evolution This will help to clarify what is arguably the most difficult aspect of NMR for students and practitioners to master

**MCAT Comprehensive Review** ,2000      **Comparative Medicine** ,2007

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