

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_2 and AX_3 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*

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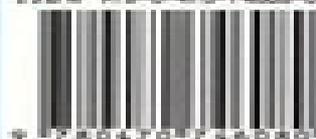


Dr James Keeler is a Senior Lecturer in Chemistry at the University of Cambridge, and a Fellow of Selwyn College. In addition to being actively involved in the development of new NMR techniques, he is also responsible for the undergraduate chemistry course, and is Editor-in-Chief of *Magnetic Resonance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

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ISBN 978-0-470-74608-0



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Understanding Nmr Spectroscopy 2nd Edition

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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

Understanding NMR Spectroscopy Ray Freeman, James Keeler, 1990
A Primer of NMR Theory with Calculations in Mathematica Alan J. Benesi, 2015-05-19
Pr sentiert die NMR Theorie in Verbindung mit Unterlagen aus Mathematica Kursen Bietet kurze Schwerpunktkapitel mit kurzen Erl uterungen zu definierten Themen und konzentriert sich dabei auf mathematische Beschreibungen Pr sentiert pr gnant wichtige Erkenntnisse aus der Quantenmechanik die bei der Prognose und Simulation

von Ergebnissen aus NMR Versuchen einfach angewendet werden können Enthält Mathematica Anleitungen die die Theorie in Form von Text Grafik Ton und Berechnungsbeispielen praktisch umsetzen Geht auf bewährte Methoden des Autors aus über 25 Jahren Lehrerfahrung zurück Die Unterlagen erläutern präzise die Theorie und bieten nützliche Berechnungsvorlagen für NMR Forscher

Modern NMR Techniques for Synthetic Chemistry Julie Fisher, 2014-10-13 A blend of theory and practical advice Modern NMR Techniques for Synthetic Chemistry illustrates how NMR spectroscopy can be used to determine the abundance size shape and function of organic molecules It provides you with a description the NMR technique used more pictorial than mathematical indicating the most common pulse sequences some practical information as appropriate followed by illustrative examples This format is followed for each chapter so you can skip the more theoretical details if the practical aspects are what interest you Following a discussion of basic parameters the book describes the utility of NMR in detecting and quantifying dynamic processes with particular emphasis on the usefulness of saturation transfer STD techniques It details pulsed field gradient approaches to diffusion measurement diffusion models and approaches to inorganic nuclei detection important as many synthetic pathways to new organics involve heavier elements The text concludes with coverage of applications of NMR to the analysis of complex mixtures natural products carbohydrates and nucleic acids all areas of activity for researchers working at the chemistry life sciences interface The book's unique format provides some theoretical insight into the NMR technique used indicating the most common pulse sequences The book draws upon several NMR methods that are resurging or currently hot in the field and indicates the specific pulse sequence used by various spectrometer manufacturers for each technique It examines the analysis of complex mixtures a feature not found in most books on this topic

The Organic Chemistry of Drug Design and Drug Action Richard B. Silverman, Mark W. Holladay, 2014-03-29 The Organic Chemistry of Drug Design and Drug Action Third Edition represents a unique approach to medicinal chemistry based on physical organic chemical principles and reaction mechanisms that rationalize drug action which allows reader to extrapolate those core principles and mechanisms to many related classes of drug molecules This new edition includes updates to all chapters including new examples and references It reflects significant changes in the process of drug design over the last decade and preserves the successful approach of the previous editions while including significant changes in format and coverage This text is designed for undergraduate and graduate students in chemistry studying medicinal chemistry or pharmaceutical chemistry research chemists and biochemists working in pharmaceutical and biotechnology industries Updates to all chapters including new examples and references Chapter 1 Introduction Completely rewritten and expanded as an overview of topics discussed in detail throughout the book Chapter 2 Lead Discovery and Lead Modification Sections on sources of compounds for screening including library collections virtual screening and computational methods as well as hit to lead and scaffold hopping expanded sections on sources of lead compounds fragment based lead discovery and molecular graphics and deemphasized solid phase synthesis and combinatorial chemistry Chapter 3

Receptors Drug receptor interactions cation π and halogen bonding atropisomers case history of the insomnia drug suvorexant Chapter 4 Enzymes Expanded sections on enzyme catalysis in drug discovery and enzyme synthesis Chapter 5 Enzyme Inhibition and Inactivation New case histories for competitive inhibition the epidermal growth factor receptor tyrosine kinase inhibitor erlotinib and Abelson kinase inhibitor imatinib for transition state analogue inhibition the purine nucleoside phosphorylase inhibitors forodesine and DADMe ImmH as well as the mechanism of the multisubstrate analog inhibitor isoniazid for slow tight binding inhibition the dipeptidyl peptidase 4 inhibitor saxagliptin Chapter 7 Drug Resistance and Drug Synergism This new chapter includes topics taken from two chapters in the previous edition with many new examples Chapter 8 Drug Metabolism Discussions of toxicophores and reactive metabolites Chapter 9 Prodrugs and Drug Delivery Systems Discussion of antibody drug conjugates

High-Resolution NMR Techniques in Organic Chemistry Timothy D.W. Claridge, 2016-04-22 High Resolution NMR Techniques in Organic Chemistry Third Edition describes the most important NMR spectroscopy techniques for the structure elucidation of organic molecules and the investigation of their behaviour in solution Appropriate for advanced undergraduate and graduate students research chemists and NMR facility managers this thorough revision covers practical aspects of NMR techniques and instrumentation data collection and spectrum interpretation It describes all major classes of one and two dimensional NMR experiments including homonuclear and heteronuclear correlations the nuclear Overhauser effect diffusion measurements and techniques for studying protein ligand interactions A trusted authority on this critical expertise High Resolution NMR Techniques in Organic Chemistry Third Edition is an essential resource for every chemist and NMR spectroscopist

Bioactive Natural Products Steven M. Colegate, Russell J. Molyneux, 2007-12-14 Following the successful format of the original this new edition presents applications of the most recent techniques for the detection isolation and structural determination of bioactive natural products It features new case studies and illustrations that demonstrate applications of techniques covered in the book Complementing as much as replacing the first edition most of the contributors are new The text includes updates on chemical extraction and NMR based structure determination and new contributions on liquid chromatography linked with mass and NMR spectroscopy dereplication approaches assessment of source material for natural products and novel bioassay development

A Practical Guide to Understanding the NMR of Polymers Peter A. Mirau, 2005 Publisher Description

Comprehensive Organometallic Chemistry III D. M. P. Mingos, Robert Crabtree, 2006-12-26 Comprehensive Organometallic Chemistry COMC III Third Edition 13 Volume Set is aimed at the specialist and non specialist alike It covers the major developments in the field in a carefully presented way with extensive cross references COMC III provides a clear and comprehensive overview of developments since 1993 and attempts to predict trends in the field over the next ten years Applications of organometallic chemistry continue to expand and this has been reflected by the significant increase in the number of volumes devoted to applications in COMC III Organic chemists have edited the volumes on organometallic

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Introduction to Polymer Chemistry, Second Edition Charles E. Carraher Jr., 2010-01-12 With an emphasis on the environment and green chemistry and materials this second edition offers detailed coverage of natural and synthetic giant molecules inorganic and organic polymers elastomers adhesives coatings fibers plastics ceramics and more

Structure, 2007

The Student's Lab Companion John W. Lehman, 2008 This comprehensive lab companion provides enough theory to help students understand how and why an operation works but emphasizes the practical aspects of an operation to help them perform the operation successfully in the lab For undergraduate or graduate students taking organic chemistry lab This comprehensive lab companion provides enough theory to help students understand how and why an operation works but emphasizes the practical aspects of an operation to help them perform the operation successfully in the lab The Second Edition makes substantive revisions of many operations to clarify existing material and add new information More environmentally friendly i.e. green lab experiments are encouraged Ideal for professors who write their own lab experiments or would like custom labs but need a source for lab operations and safety information

Acta Chimica Hungarica, 1985

Two-dimensional NMR Spectroscopy William R. Croasmun, Robert M. K. Carlson, 1994

American Book Publishing Record, 2005

Chemistry and Industry, 2002

Choice, 2006

The Use of Ab Initio Calculations and NMR Relaxation Time Experiments to Obtain Molecular Structure and Dynamic Information of Systems in Solution Jon David Trudeau, 1993

Comprehensive Desk Reference of Polymer Characterization and Analysis Robert F. Brady, 2003 This book is a practical manual for those who analyze polymers Self contained chapters describe when a technique should be selected explain its basic principles describe how instruments are constructed and operated and teach how the data obtained relate to molecular structure and physical properties Many clear illustrations are included Implicit memory refers to a change in task performance due to an earlier experience that is not consciously remembered This book is not a research manual but rather a guide to performing and understanding polymer characterization and an introduction to the specialized literature of the analytical chemistry of polymers The techniques covered are directly relevant to the characterization of synthetic polymers such as adhesives sealants polymers composites

coatings elastomers rubber and other nonmetallic materials Many techniques are also quite useful for natural and biological polymers

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Table of Contents Understanding Nmr Spectroscopy 2nd Edition

1. Understanding the eBook Understanding Nmr Spectroscopy 2nd Edition
 - The Rise of Digital Reading Understanding Nmr Spectroscopy 2nd Edition
 - Advantages of eBooks Over Traditional Books
2. Identifying Understanding Nmr Spectroscopy 2nd Edition
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Understanding Nmr Spectroscopy 2nd Edition
 - User-Friendly Interface
4. Exploring eBook Recommendations from Understanding Nmr Spectroscopy 2nd Edition
 - Personalized Recommendations
 - Understanding Nmr Spectroscopy 2nd Edition User Reviews and Ratings

- Understanding Nmr Spectroscopy 2nd Edition and Bestseller Lists
- 5. Accessing Understanding Nmr Spectroscopy 2nd Edition Free and Paid eBooks
 - Understanding Nmr Spectroscopy 2nd Edition Public Domain eBooks
 - Understanding Nmr Spectroscopy 2nd Edition eBook Subscription Services
 - Understanding Nmr Spectroscopy 2nd Edition Budget-Friendly Options
- 6. Navigating Understanding Nmr Spectroscopy 2nd Edition eBook Formats
 - ePub, PDF, MOBI, and More
 - Understanding Nmr Spectroscopy 2nd Edition Compatibility with Devices
 - Understanding Nmr Spectroscopy 2nd Edition Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Understanding Nmr Spectroscopy 2nd Edition
 - Highlighting and Note-Taking Understanding Nmr Spectroscopy 2nd Edition
 - Interactive Elements Understanding Nmr Spectroscopy 2nd Edition
- 8. Staying Engaged with Understanding Nmr Spectroscopy 2nd Edition
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Understanding Nmr Spectroscopy 2nd Edition
- 9. Balancing eBooks and Physical Books Understanding Nmr Spectroscopy 2nd Edition
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Understanding Nmr Spectroscopy 2nd Edition
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Understanding Nmr Spectroscopy 2nd Edition
 - Setting Reading Goals Understanding Nmr Spectroscopy 2nd Edition
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Understanding Nmr Spectroscopy 2nd Edition
 - Fact-Checking eBook Content of Understanding Nmr Spectroscopy 2nd Edition
 - Distinguishing Credible Sources

13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
 - Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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