

# 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*

*"...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*

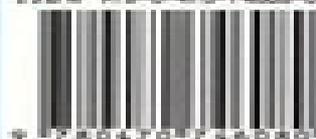


**Dr James Keeler** is a Senior Lecturer in Chemistry at the University of Cambridge, and a Fellow of Selwyn College. In addition to being actively involved in the development of new NMR techniques, he is also responsible for the undergraduate chemistry course, and is Editor-in-Chief of *Magnetic Resonance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

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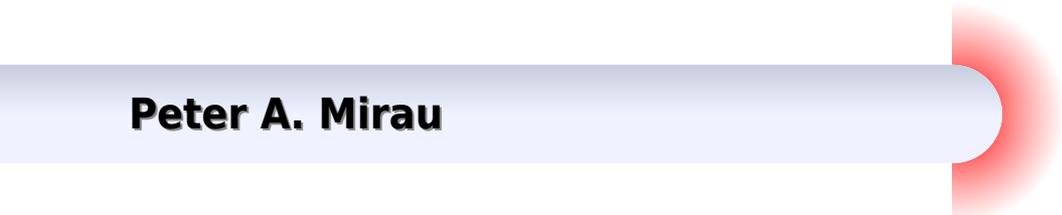
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# Understanding Nmr Spectroscopy 2nd Edition

**Peter A. Mirau**



## **Understanding Nmr Spectroscopy 2nd Edition:**

Understanding NMR Spectroscopy James Keeler, 2010-05-24 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* 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 **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 *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  $\pi$  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

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**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 chemistry towards organic synthesis this is now organized by reaction type so as to be readily accessible to the organic community Like its predecessors COMC 1982 and COMC II 1995 this new work is the essential reference text for any chemist or technologist who needs to use or apply organometallic compounds Also available online via ScienceDirect 2006 featuring extensive browsing searching and internal cross referencing between articles in the work plus dynamic linking to journal articles and abstract databases making navigation flexible and easy For more information pricing options and availability visit [www.info.sciencedirect.com](http://www.info.sciencedirect.com) Presents a comprehensive overview of the major developments in the field since 1993 providing general and significant insights Highlights the expansion of applications in organometallic chemistry with a strong organic synthesis focus Provides a structured first point of entry to the key literature and background material for those planning research teaching and writing about the area

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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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