

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*

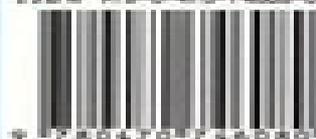


Dr James Keeler is a Senior Lecturer in Chemistry at the University of Cambridge, and a Fellow of Selwyn College. In addition to being actively involved in the development of new NMR techniques, he is also responsible for the undergraduate chemistry course, and is Editor-in-Chief of *Magnetic Resonance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

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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

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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

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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 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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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 *Two-dimensional NMR Spectroscopy* William R. Croasmun, Robert M. K. Carlson, 1994 *Acta Chimica Hungarica*, 1985 *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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