

# Introduction to **Solid-State NMR Spectroscopy**

Melinda J. Duer

This book 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.

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**Introduction to Solid-State NMR Spectroscopy**

Melinda J. Duer, 2005-07-29 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

**Solid State NMR** Klaus

Müller, Marco Geppi, 2021-06-23 Solid State NMR A thorough and comprehensive textbook covering the theoretical background experimental approaches and major applications of solid state NMR spectroscopy Nuclear Magnetic Resonance NMR spectroscopy is a powerful non destructive technique capable of providing information about the molecular structure and dynamics of molecules Alongside solution state NMR a well established technique to study chemical structures and investigate physico chemical properties of molecules in solutions solid state NMR SSNMR offers many exciting possibilities for the analysis of solid and soft materials across scientific fields SSNMR shows unique capabilities for a detailed investigation of structural and dynamic properties of materials over wide space and time ranges For this reason and thanks to significant advances in the past several years the application of SSNMR to materials is rapidly increasing in disciplines such as chemistry physics and materials and life sciences Solid State NMR Principles Methods and Applications offers a systematic introduction to the theory methodological concepts and major experimental methods of SSMR spectroscopy Exploring the unique potential of SSNMR for the structural and dynamic characterization of soft and either amorphous or crystalline solid materials this comprehensive textbook provides foundational knowledge and recent developments of SSNMR covering physical and theoretical background experimental methods and applications to pharmaceuticals polymers inorganic and hybrid materials liquid crystals and model membranes Written by two expert authors to ensure a clear and consistent presentation of the subject this textbook Includes a brief introduction to the historical aspects and broad theoretical background of solid state NMR spectroscopy Provides helpful illustrations to explain the various SSNMR concepts and methods Features accessible descriptive text with self consistent use of quantum mechanics Covers the experimental aspects

of SSNMR spectroscopy and in particular a description of many useful pulse sequences Contains references to relevant literature Solid State NMR Principles Methods and Applications is the ideal textbook for university courses on SSNMR advanced spectroscopies and a valuable single volume reference for spectroscopists chemists and researchers in the field of materials

**Solid-State NMR** David C. Apperley, Robin K. Harris, Paul Hodgkinson, 2012-06-10 The power of nuclear magnetic resonance NMR for characterizing molecules dissolved in solution is widely acknowledged and NMR forms an essential component of undergraduate chemistry degrees However the application of NMR to the solid state is much less well appreciated This text sets out the fundamental principles of solid state NMR explaining how NMR in solids differs from that in solution showing how the various interactions of NMR can be manipulated to yield high resolution spectra and to give information on local structure and dynamics in solids This book aims to take some of the mystique out of solid state NMR by providing a comprehensible discussion of the methodology including the basic concepts and a practical guide to implementation of the experiments A basic knowledge of solution state NMR is assumed and is only briefly covered The text is intended for those in academia and industry expecting to use solid state NMR in their research and looking for an accessible introduction to the field It will also be valuable for non experts interested in learning how NMR can be usefully applied to solid systems Detailed mathematical treatments are delayed to a chapter at the mid point of the text and can be skipped Introductions to experiments and numerical simulations are provided to help link NMR results to experimental practice The different aspects of solid state NMR from basic pulse and acquire experiments to sophisticated techniques for the measurement of anisotropy information are presented Examples illustrate the wide variety of applications of the technique and its complementarity to other solid state characterization techniques such as X ray diffraction Various aspects of NMR crystallography are covered as are topics of motion in solids

Solid State NMR Spectroscopy Melinda J. Duer, 2008-04-15 This book is for those familiar with solution state NMR who are encountering solid state NMR for the first time It presents the current understanding and applications of solid state NMR with a rigorous but readable approach making it easy for someone who merely wishes to gain an overall impression of the subject without details This dual requirement is met through careful construction of the material within each chapter The book is divided into two parts Fundamentals and Further Applications The section on Fundamentals contains relatively long chapters that deal with the basic theory and practice of solid state NMR The essential differences and extra scope of solid state NMR over solution state is dealt with in an introductory chapter The basic techniques that all chapters rely on are collected into a second chapter to avoid unnecessary repetition later Remaining chapters in the Fundamentals part deal with the major areas of solid state NMR which all solid state NMR spectroscopists should know about Each begins with an overview of the topic that puts the chapter in context The basic principles upon which the techniques in the chapter rely are explained in a separate section Each of these chapters exemplifies the principles and techniques with the applications most commonly found in current

practice The Further Applications section contains a series of shorter chapters which describe the NMR techniques used in other more specific areas The basic principles upon which these techniques rely will be expounded only if not already in the Fundamentals part

*Solid-State NMR I Methods* B. Blümich, 2012-12-06 1 A R Grimmer Berlin FRG B Bl mich Aachen FRG Introduction to Solid State NMR 2 F Laupretre Paris France High Resolution <sup>13</sup>C NMR Investigations of Local Dynamics in Bulk Polymers at Temperatures Below and Above the Glass Transition Temperature 3 D Raftery Philadelphia PA B F Chmelka Santa Barbara CA Xenon NMR Spectroscopy 4 G Fleischer Leipzig FRG F Fajara Mainz FRG NMR as a Generalized Incoherent Scattering Experiment 5 P Bl mler B Bl mich Mainz FRG NMR Imaging of Solids

**Nuclear Magnetic Resonance** G. A. Webb, 2005 As a spectroscopic method nuclear magnetic resonance NMR has seen spectacular growth over the past two decades both as a technique and in its applications Today the applications of NMR span a wide range of scientific disciplines from physics to biology to medicine Each volume of Nuclear Magnetic Resonance comprises a combination of annual and biennial reports which together provide comprehensive coverage of the literature on this topic This Specialist Periodical Report reflects the growing volume of published work involving NMR techniques and applications in particular NMR of natural macromolecules which is covered in two reports NMR of Proteins and Nucleic Acids and NMR of Carbohydrates Lipids and Membranes For those wanting to become rapidly acquainted with specific areas of NMR this title provides unrivalled scope of coverage Seasoned practitioners of NMR will find this an invaluable source of current methods and applications Volume 34 covers literature published from June 2003 to May 2004 Specialist Periodical Reports provide systematic and detailed review coverage in major areas of chemical research Compiled by teams of leading authorities in the relevant subject areas the series creates a unique service for the active research chemist with regular in depth accounts of progress in particular fields of chemistry Subject coverage within different volumes of a given title is similar and publication is on an annual or biennial basis

*A Complete Introduction to Modern NMR Spectroscopy* Roger S. Macomber, 1997-12-23 Clear accessible coverage of modern NMR spectroscopy for students and professionals in many fields of science Nuclear magnetic resonance NMR spectroscopy has made quantum leaps in the last decade becoming a staple tool in such divergent fields as chemistry physics materials science biology and medicine That is why it is essential that scientists working in these areas be fully conversant with current NMR theory and practice This down to basics text offers a comprehensive up to date treatment of the fundamentals of NMR spectroscopy Using a straightforward approach that develops all concepts from a rudimentary level without using heavy mathematics it gives readers the knowledge they need to solve any molecular structure problem from a complete set of NMR data Topics are illustrated throughout with hundreds of figures and actual spectra Chapter end summaries and review problems with answers are included to help reinforce and test understanding of key material From NMR studies of biologically important molecules to magnetic resonance imaging this book serves as an excellent all around primer on NMR spectroscopic analysis

**Solid-State Properties of**

**Pharmaceutical Materials** Stephen R. Byrn, George Zograf, Xiaoming (Sean) Chen, 2017-08-28 Presents a detailed discussion of important solid state properties methods and applications of solid state analysis Illustrates the various phases or forms that solids can assume and discusses various issues related to the relative stability of solid forms and tendencies to undergo transformation Covers key methods of solid state analysis including X ray powder diffraction thermal analysis microscopy spectroscopy and solid state NMR Reviews critical physical attributes of pharmaceutical materials mainly related to drug substances including particle size surface area hygroscopicity mechanical properties solubility and physical and chemical stability Showcases the application of solid state material science in rational selection of drug solid forms analysis of various solid forms within drug substance and the drug product and pharmaceutical product development Introduces appropriate manufacturing and control procedures using Quality by Design and other strategies that lead to safe and effective products with a minimum of resources and time

**NMR Spectroscopy in Pharmaceutical Analysis** Iwona Wawer, Bernd Diehl, 2017-07-07 For almost a decade quantitative NMR spectroscopy qNMR has been established as valuable tool in drug analysis In all disciplines i e drug identification impurity profiling and assay qNMR can be utilized Separation techniques such as high performance liquid chromatography gas chromatography super fluid chromatography and capillary electrophoresis techniques govern the purity evaluation of drugs However these techniques are not always able to solve the analytical problems often resulting in insufficient methods Nevertheless such methods find their way into international pharmacopoeias Thus the aim of the book is to describe the possibilities of qNMR in pharmaceutical analysis Beside the introduction to the physical fundamentals and techniques the principles of the application in drug analysis are described quality evaluation of drugs polymer characterization natural products and corresponding reference compounds metabolism and solid phase NMR spectroscopy for the characterization drug substances e g the water content polymorphism and drug formulations e g tablets powders This part is accompanied by more special chapters dealing with representative examples They give more detailed information by means of concrete examples Combines theory techniques and concrete applications all of which closely resemble the laboratory experience Considers international pharmacopoeias addressing the concern for licensing Features the work of academics and researchers appealing to a broad readership

**Annual Reports on NMR Spectroscopy** Graham A. Webb, 2012-12-31 Nuclear magnetic resonance NMR is an analytical tool used by chemists and physicists to study the structure and dynamics of molecules In recent years no other technique has gained such significance as NMR spectroscopy It is used in all branches of science in which precise structural determination is required and in which the nature of interactions and reactions in solution is being studied Annual Reports on NMR Spectroscopy has established itself as a premier means for the specialist and non specialist alike to become familiar with new techniques and applications of NMR spectroscopy Annual Reports on NMR Spectroscopy has established itself as a premier means for the specialist and non specialist alike to become familiar with new techniques and applications of NMR spectroscopy

**Modern Methods in**

**Solid-state NMR** Paul Hodgkinson, 2018-04-05 Solid state NMR covers an enormous range of material types and experimental techniques. Although the basic instrumentation and techniques of solids NMR are readily accessible, there can be significant barriers even for existing experts to exploring the bewildering array of more sophisticated techniques. In this unique volume, a range of experts in different areas of modern solid state NMR explain about their area of expertise, emphasising the practical aspects of implementing different techniques and illustrating what questions can and cannot be addressed. Later chapters address complex materials, showing how different NMR techniques discussed in earlier chapters can be brought together to characterise important materials types. The volume as a whole focusses on topics relevant to the developing field of NMR crystallography, the use of solids NMR as a complement to diffraction crystallography. This book is an ideal complement to existing introductory texts and reviews on solid state NMR. New researchers wanting to understand new areas of solid state NMR will find each chapter to be the equivalent to spending time in the laboratory of an internationally leading expert, learning the hints and tips that make the difference between knowing about a technique and being ready to put it into action. With no equivalent on the market, it will be of interest to every solid state NMR researcher, academic and postgraduate working in the chemical sciences.

**Solid State Nuclear Magnetic Resonance** David E. Axelson, 2012-03-29 Solid state nuclear magnetic resonance now offers a wide variety of methods for characterization of materials of different compositions over a wide range of experimental conditions, temperatures, pressures, etc. Both simple and sophisticated pulse sequences enable one to selectively probe and quantify physical properties of interest. This book mainly dwells on the practical aspects of selected topics and uses a largely non-mathematical, although extensively referenced, approach to the introduction of solid state NMR concepts. Chapter 1 Principles of Solid State NMR, Chapter 2 Introduction to Pulse Sequences, Chapter 3 Decoupling, Chapter 4 Quantitative Analysis, Chapter 5 Artifacts, Chapter 6 Line Broadening Mechanisms, Chapter 7 Resolution Enhancement, Chapter 8 Variable Temperature.

**NMR Spectroscopy of Biological Solids** A. Ramamoorthy, 2005-09-22 Over the past decade, a myriad of techniques have shown that solid state nuclear magnetic resonance NMR can be used in a broad spectrum of applications with exceptionally impressive results. Solid state NMR results can yield high resolution details on the structure and function of many important biological solids, including viruses, fibril-formin.

The Chemistry of Organolithium Compounds Zvi Rappoport, Ilan Marek, 2004-08-20 This is the first volume in the series to concentrate on organolithium compounds, the sub-series 'The chemistry of the metal-carbon bond'. 5 vols. Treats organometallics in general. It deals with theoretical, physical, computational aspects as well as major spectroscopies such as MS, NMR, IR, UV, etc. and both biological and industrial applications. The core of the volume is the synthetic chapters with lots of examples for modern synthetic approaches. Written by key researchers in the field. An invaluable reference source to organic chemists working in academia and industry. Features important reagents in organic synthesis.

**Handbook of Thin Films** Hari Singh Nalwa, 2001-11-17 This five-volume handbook focuses on processing

techniques characterization methods and physical properties of thin films thin layers of insulating conducting or semiconductor material The editor has composed five separate thematic volumes on thin films of metals semimetals glasses ceramics alloys organics diamonds graphites porous materials noncrystalline solids supramolecules polymers copolymers biopolymers composites blends activated carbons intermetallics chalcogenides dyes pigments nanostructured materials biomaterials inorganic polymer composites organoceramics metallocenes disordered systems liquid crystals quasicrystals and layered structures Thin films is a field of the utmost importance in today's materials science electrical engineering and applied solid state physics with both research and industrial applications in microelectronics computer manufacturing and physical devices Advanced high performance computers high definition TV digital camcorders sensitive broadband imaging systems flat panel displays robotic systems and medical electronics and diagnostics are but a few examples of miniaturized device technologies that depend the utilization of thin film materials The Handbook of Thin Films Materials is a comprehensive reference focusing on processing techniques characterization methods and physical properties of these thin film materials

*Advances in Magnetic Resonance* Warren S. Warren, 2012-12-02 *Advances in Magnetic Resonance* The Waugh Symposium Volume 14 is a collection of manuscripts presented at the 1989 symposium on High Resolution NMR in Solids held at the Massachusetts Institute of Technology The contributors provide 20 to 30 page articles consistent with AMR's traditional emphasis on quantitative analysis of NMR techniques Organized into 13 chapters this book discusses the principles triple quantum filtered two dimensional exchange spectroscopy and its application in the measurement of cross correlation between pairs of dipole dipole interactions It then describes alternative ways of using fictitious spin in pulsed nuclear quadrupole resonance or NMR General topics on the application of optical spectroscopy the saturation of spin spin energy by slow continuous bulk rotation the frequency switched Lee Goldburg pulse cycle and high resolution proton NMR in solid systems are also explored A chapter examines an entirely different view of spin dynamics in the presence of radio frequency fields This book also deals with the theoretical background and application of solid state and zero field NMR spectroscopies to structure determination Lastly the utilization of the Floquet formalism in the design of broadband propagators in two level systems and the two classes of novel NMR phenomena related to the symmetrization postulate are discussed Analytical and quantum chemists physicists biochemists and materials science researchers will find this book invaluable

*Experimental Approaches of NMR Spectroscopy* The Nuclear Magnetic Resonance Society of Japan, 2017-11-23 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

**Structure and Performance of Cements** P. Barnes, J. Bensted, 2002-11-01 Drawing together a multinational team of authors this second edition of Structure and Performance of Cements highlights the latest global advances in the field of cement technology Three broad categories are covered basic materials and methods cement extenders and techniques of examination Within these categories consideration has been given

Spectroscopy of Emerging Materials Eric C. Faulques, Dale L. Perry, Andrei V. Yermenko, 2006-01-14 A comprehensive discussion of the key role of modern spectroscopic investigations in interdisciplinary materials science and engineering covering emerging materials that are either absolutely novel or well known materials with recently discovered exciting properties The types of spectroscopy discussed include optical electronic and magnetic UV visible absorption Rayleigh scattering photoluminescence vibrational magnetic resonance electron energy loss EXAFS XANES optical tomography time resolved spectroscopy and point contact spectroscopy The materials studied are highly topical with a focus on carbon and silicon nanomaterials including nanotubes fullerenes nanoclusters metallic superconducting phases molecular materials magnetic and charge stripe oxides and biomaterials Theoretical treatments are presented of molecular vibrational dynamics vibration induced decay of electronic excited states nanoscale spin orbit coupling in 2D Si based structures and the growth of semiconductor clusters

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