



Solid-State Nmr I: Methods: 001 (N M R, Basic Principles and Progress)

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Solid State Nmr I Methods Nmr Basic Principles And Progress Vol 3

Anne E. McDermott, Tatyana Polenova



Solid State Nmr I Methods Nmr Basic Principles And Progress Vol 3:

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 ¹³C 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 Fajarsa 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 Volume 3 R. K. Harris, 1972 Annotation 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 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 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 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 Solid-State NMR III Organic Matter Bernhard Blümich, 2012-12-06 Solid State NMR is a branch of Nuclear Magnetic Resonance which is presently experiencing a phase of strongly increasing popularity The most striking evidence is the large number of contributions from Solid State Resonance at NMR meetings approaching that of liquid state resonance Important progress can be observed in three areas Methodological developments applications to inorganic matter and applications to organic matter These developments are intended to be captured in three volumes in this series each of them being devoted to more or less one of these areas The present volume on Solid State NMR III is devoted mainly to organic matter The recent developments of deuterium NMR and their applications are reviewed in the first chapter Crosspolarization MAS and dynamic angle spinning are being explored for enhancement of information and sensitivity In addition to the analysis of classical relaxation times and modern 2D spectra detailed dynamic information becomes accessible from investigations of the relaxation time anisotropies The second chapter examines cross polarization in static and rotating solids under conditions of spin diffusion and thermal motion The underlying dipole dipole interaction is further exploited by the techniques described in the third chapter for studies of polymer polymer miscibility Short range techniques are discriminated from long range techniques based on spin diffusion The use of these

techniques is illustrated by a case study of PMMA/PVF blends. The last chapter addresses novel methods and applications of two dimensional exchange NMR for investigations of relative molecular orientations, polymer morphology, molecular dynamics and macroscopic molecular order. *Solid-State NMR IV Methods and Applications of Solid-State NMR B.*

Blümich, 2012-12-06. Solid State NMR is a branch of Nuclear Magnetic Resonance which is presently experiencing a phase of strongly increasing popularity. The most striking evidence is the large number of contributions from Solid State Resonance at NMR meetings approaching that of liquid state resonance. Important progress can be observed in the areas of methodological developments and applications to organic and inorganic matter. One volume devoted to more or less one of each of these areas has been published in the preceding three issues. This volume can be considered an addendum to this series. Selected methods and applications of Solid State NMR are featured in three chapters. The first one treats the recoupling of dipolar interactions in solids which are averaged by fast sample rotation. Following an introduction to effective Hamiltonians and Floquet theory, different types of experiment such as rotary resonance, dipolar chemical shift correlation spectroscopy, rotational resonance and multipulse recoupling are treated in the powerful Floquet formalism. In the second chapter, the different approaches to line narrowing of quadrupolar nuclei are reviewed in a consistent formulation of double resonance, DARR and dynamic angle spinning (DAS). Practical aspects of probe design are considered as well as advanced 2D experiments, sensitivity enhancement techniques and spinning sideband manipulations. The use of such techniques dramatically increases the number of nuclei which can be probed in high resolution NMR spectroscopy. The final chapter describes new experimental approaches and results of structural studies of noncrystalline solids. *Solid-State NMR II B.*

Blümich, 2013-03-09. 1. G. Engelhardt, H. Koller, Stuttgart, FRG. ²⁹Si NMR of Inorganic Solids. 2. H. Pfeifer, Leipzig, FRG. NMR of Solid Surfaces. 3. A. Sebald, Bayreuth, FRG. MAS and CP MAS NMR of Less Common Spin 1/2 Nuclei. 4. C. Jäger, Mainz, FRG. Satellite Transition Spectroscopy of Quadrupolar Nuclei. 5. D. Brinkmann, M. Mali, Zürich, CH. NMR NQR Studies of High Temperature Superconductors. **Nuclear Magnetic Resonance**. R. K. Harris, 2007-10-31. 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 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. 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

Deuterium and Shift Calculation ,2012-12-06 In 1931 Vrey Brickwedde and Murphy discovered the hydrogen isotope deuterium The isotopic enrichment was found to arise from the fact that the electrolysis of light water is faster than of heavy water 1 2 This success showed that although different isotopes of an element behave identically from a chemical standpoint the different isotopic masses nevertheless lead to both isotope effects on equilibrium as well as on rate constants of chemical reactions Soon ratios of equilibrium constants of isotopic reactions were called equilibrium isotope effects EIE ratios of isotopic rate constants kinetic isotope effects KIE Isotope effects have been found to be especially large for those elements which are directly involved in bond breaking and bond formation during the reaction studied 3 Such effects are therefore referred to as primary Isotopic substitution in atomic sites which maintain all chemical bonds with their neighbors during the reaction of interest leads then only to smaller secondary isotope effects Because of the unique mass relation between the different hydrogen isotopes hydrogen deuterium isotope effects are particularly large and have attracted most attention The largest contributions to these effects arise from changes in the vibrational frequencies of the reactants The theory of equilibrium isotope effects has been founded by Vrey 4 and Bigeleisen 5 6 and has widely been accepted 3

NMR of Quadrupolar Nuclei in Solid Materials Roderick E. Wasylshen, Sharon E. Ashbrook, Stephen Wimperis, 2012-12-19 NMR OF QUADRUPOLEAR NUCLEI IN SOLID MATERIALS Over the past 20 years technical developments in superconducting magnet technology and instrumentation have increased the potential of NMR spectroscopy so that it is now possible to study a wide range of solid materials In addition one can probe the nuclear environments of many other additional atoms that possess the property of spin In particular it is possible to carry out NMR experiments on isotopes that have nuclear spin greater than 1/2 i.e. quadrupolar nuclei Since more than two thirds of all NMR active isotopes are quadrupolar nuclei applications of NMR spectroscopy with quadrupolar nuclei are increasing rapidly The purpose of this handbook is to provide under a single cover the fundamental principles techniques and applications of quadrupolar NMR as it pertains to solid materials Each chapter has been prepared by an expert who has made significant contributions to our understanding and appreciation of the importance of NMR studies of quadrupolar nuclei in solids The text is divided into three sections The first provides the reader with the background necessary to appreciate the challenges in acquiring and interpreting NMR spectra of quadrupolar nuclei in solids The second presents cutting edge techniques and methodology for employing these techniques to investigate quadrupolar nuclei in solids The final section explores applications of solid state NMR studies of solids ranging from investigations of dynamics characterizations of biological samples organic and inorganic materials porous materials glasses catalysts semiconductors and high temperature superconductors About EMR Handbooks The Encyclopedia of Magnetic Resonance EMR 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 EMR Handbooks on specific areas of NMR and MRI The chapters of each of these handbooks will comprise a carefully chosen selection of Encyclopedia articles In consultation with the EMR Editorial Board the EMR Handbooks are coherently planned in advance by specially selected Editors and new articles are written together with updates of some already existing articles 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 the Encyclopedia of Magnetic Resonance at your fingertips Visit www.wileyonlinelibrary.com/ref/emr

Catalysis J. R. Anderson, M. Boudart, 2012-12-06 NMR methods have for a considerable time been standard processes for the analysis of molecular structure so much so that they are now universally regarded as indispensable for this purpose Nevertheless with the passage of time NMR methodology has been elaborated to levels of ever increasing complexity and analytical sophistication so that the non specialist may now be readily excused for the belief that for anything beyond relatively elementary methods one would be well advised to work in collaboration with the specialist experts The application of NMR methods to the field of catalysis occurred in the main relatively late in the day mainly because those catalysts of greatest industrial importance that is heterogeneous catalysts are solids and so require special NMR methods if usefully narrow NMR lines are to be observable Even so magic angle spinning NMR methodology is now thoroughly well established and is finding increasing use in the study of catalyst structure Of course conventional NMR methods have been used for a considerable time for the analysis of the products of catalytic reactions Chapter 1 of the present volume by Professor Jacques Fraissard and his collaborators is designed to give an account of the application of NMR methods to the field of catalysis but not including the conventional use of NMR for reaction product analysis since this is already well covered in the existing NMR literature

Annual Reports on NMR Spectroscopy, 2003-12-18 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 grown to such importance as NMR spectroscopy It is used in all branches of science where precise structural determination is required and where the nature of interactions and reactions in solution is being studied Annual Reports on NMR has established itself as a premier means for the specialist and nonspecialist alike to become familiar with new techniques and applications of NMR spectroscopy Includes comprehensive review articles on NMR Spectroscopy NMR is used in all branches of science No other technique has grown to such importance as NMR Spectroscopy in recent years

Handbook of Solid State Chemistry, 6 Volume Set Richard Dronskowski, Shinichi Kikkawa, Andreas Stein, 2017-10-23 This most comprehensive and unrivaled compendium in the field provides an up to date account of the chemistry of solids nanoparticles and hybrid materials Following a valuable introductory chapter reviewing important synthesis techniques the

handbook presents a series of contributions by about 150 international leading experts the Who's Who of solid state science. Clearly structured in six volumes it collates the knowledge available on solid state chemistry starting from the synthesis and modern methods of structure determination. Understanding and measuring the physical properties of bulk solids and the theoretical basis of modern computational treatments of solids are given ample space as are such modern trends as nanoparticles, surface properties and heterogeneous catalysis. Emphasis is placed throughout not only on the design and structure of solids but also on practical applications of these novel materials in real chemical situations. *Solid State NMR Studies of Biopolymers* Anne E. McDermott, Tatyana Polenova, 2012-12-19. The content of this volume has been added to eMagRes formerly Encyclopedia of Magnetic Resonance, the ultimate online resource for NMR and MRI. The field of solid state NMR of biological samples ssNMR has blossomed in the past 5-10 years and a cohesive overview of the technology is needed for new practitioners in industry and academia. This title provides an overview of Solid State NMR methods for studying structure dynamics and ligand binding in biopolymers and offers an overview of RF pulse sequences for various applications including not only a systematic catalog but also a discussion of theoretical tools for analysis of pulse sequences. Practical examples of biochemical applications are included along with a detailed discussion of the many aspects of sample preparation and handling that make spectroscopy on solid proteins successful. About EMR Handbooks eMagRes Handbooks. The Encyclopedia of Magnetic Resonance up to 2012 and eMagRes from 2013 onward publish 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 EMR Handbooks eMagRes Handbooks on specific areas of NMR and MRI. The chapters of each of these handbooks will comprise a carefully chosen selection of articles from eMagRes. In consultation with the eMagRes Editorial Board, the EMR Handbooks eMagRes Handbooks are coherently planned in advance by specially selected Editors and new articles are written together with updates of some already existing articles 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. View other eMagRes publications here. **Multinuclear Magnetic Resonance in Liquids and Solids – Chemical Applications** P. Granger, Robin K. Harris, 2012-12-06. The idea of this NATO school was born during philosophical discussions with Dr Brevard on the present and future of NMR during a night walk under the palm trees in Biskra during a seminar held in this oasis. It was clear for us that the recent progress in the field of NMR, especially inverse spectroscopy and the development of MAS, was opening new perspectives for chemists. We realised also that organometallic and inorganic chemists were not clearly informed about the potentialities of all the new methods. NATO with its summer schools was offering a good opportunity to propose to the chemical community a session

where those problems would be largely developed This School is then the prolongation of the two previous ones Palermo in 1976 on the less receptive nuclei and Stirling in 1982 on the multinuclear approach to NMR spectroscopy It was divided into two sub sessions NMR in the liquid state and NMR in the solid state This is reflected in the book organization As indicated by the title of this School we were mainly concerned with the methodological aspects of multinuclear NMR If many examples are given they appear only as a support for the understanding of the theory or in explanation of some practical aspects of the different experiments Each domain is introduced by a lecture which presents selected examples

Nuclear Magnetic Resonance Volume 4 R. K. Harris, 1972 Annotation 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 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 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 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

Ab Initio Calculations of Conformational Effects on ^{13}C NMR Spectra of Amorphous Polymers R. Born, H.W. Spiess, 2012-12-06 In NMR it is well known that the chemical shift conveys structural information e.g. a carbonyl carbon will have a resonance frequency appreciably different from a methyl carbon etc The relation between structure and chemical shift is mostly established by empirical rules on the basis of prior experience It is only quite recently that the advent of both comparatively cheap computing power and novel quantum chemistry approaches have provided feasible routes to calculate the chemical shift at the ab initio level for molecules of reasonable size This raises the question whether application of these novel theoretical concepts offers a means of obtaining new structural information for the complex chain molecules one deals with in polymer science Solid state ^{13}C NMR spectra of glassy amorphous polymers display broad partially structured resonance regions that reflect the underlying disorder of the polymer chains The chemical shift responds to the variation of the geometry of the chain and the broad resonance regions can be explained by an inhomogeneous superposition of various chain geometries and thus chemical shifts In this review we present a novel approach to combine polymer chain statistical models quantum chemistry and solid state NMR to provide quantitative information about the local chain geometry in amorphous polymers The

statistical model yields the relative occurrence of the various geometries and quantum chemistry together with a force field geometry optimization establishes the link between geometry and chemical shift *Encyclopedia of Supramolecular Chemistry - Two-Volume Set (Print)* Jerry L. Atwood, Jonathan W. Steed, 2013-10-09 The two volume Encyclopedia of Supramolecular Chemistry offers authoritative centralized information on a rapidly expanding interdisciplinary field User friendly and high quality articles parse the latest supramolecular advancements and methods in the areas of chemistry biochemistry biology environmental and materials science and engineering physics computer science and applied mathematics Designed for specialists and students alike the set covers the fundamentals of supramolecular chemistry and sets the standard for relevant future research **Nuclear Magnetic Resonance in Modern Technology** G.E.

Maciel, 2012-12-06 This volume represents the primary lectures of the NATO Advanced Study Institute ASI on Nuclear Magnetic Resonance in Modern Technology which was held at Sarigerme Park near the Dalaman Airport on the southern Aegean shore of Turkey from August 23 to September 4 1992 As indicated in the title this ASI was aimed at examining displaying and perhaps influencing the role of nuclear magnetic resonance NMR in modern technological activity The lectures summarized in this volume and the numerous short contributed talks and posters were primarily aimed at the question What is NMR doing in support of modern technology During the main discussion periods and the numerous small scheduled meetings of specific interest groups this same topic was also addressed along with questions like What could or should NMR be doing in support of modern technology With this kind of subject orientation the organizers attempted to include a large participation at the ASI from scientists and engineers from diverse private industries in which NMR does or perhaps should play a substantial role in supporting or optimizing technology Perhaps because of a combination of worldwide industrial contractions and residual corporate nervousness regarding the then recent Gulf War which caused a one year postponement of this ASI the participation from private industry was numerically disappointing We hope that this book will serve to bring the role of NMR in modern industry to the attention of numerous industrial scientists and engineers who were unable to attend the AS **Annual Reports on NMR Spectroscopy** Graham A. Webb, 2006-03-15 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 grown to such importance as NMR spectroscopy It is used in all branches of science where precise structural determination is required and where the nature of interactions and reactions in solution is being studied Annual Reports on NMR has established itself as a premier means for the specialist and nonspecialist alike to become familiar with new techniques and applications of NMR spectroscopy Includes comprehensive review articles on NMR Spectroscopy Provides nonspecialists using this technology in all branches of science with the latest developments in the field Keeps specialists up to date on the newest techniques in this important and fast changing field **Pore Structure of Cement-Based Materials** Kalliopi K. Aligizaki, 2005-09-22 Pore Structure of Cement Based Materials provides a thorough

treatment of the experimental techniques used to characterize the pore structure of materials The text presents the principles and practical applications of the techniques used organized in an easy to follow and uncomplicated manner providing the theoretical background the way to analyze experimental data and the factors affecting the results The book is the single comprehensive source of the techniques most commonly used for pore structure analysis covering simple techniques like mercury intrusion porosimetry and water absorption to the more sophisticated small angle scattering and nuclear magnetic resonance The book is an essential reference text for researchers users and students in materials science applied physics and civil engineering who seek a deep understanding of the principles and limitations of the techniques used for pore structure analysis of cement based materials NMR Crystallography Robin K. Harris, Roderick E.

Wasylishen, Melinda J. Duer, 2012-12-19 The content of this volume has been added to eMagRes formerly Encyclopedia of Magnetic Resonance the ultimate online resource for NMR and MRI The term NMR Crystallography has only recently come into common usage and even now causes raised eyebrows within some parts of the diffraction community The power of solid state NMR to give crystallographic information has considerably increased since the CPMAS suite of techniques was introduced in 1976 In the first years of the 21st century the ability of NMR to provide information to support and facilitate the analysis of single crystal and powder diffraction patterns has become widely accepted Indeed NMR can now be used to refine diffraction results and in favorable cases to solve crystal structures with minimal or even no diffraction data The increasing ability to relate chemical shifts including the tensor components to the crystallographic location of relevant atoms in the unit cell via computational methods has added significantly to the practice of NMR crystallography Diffraction experts will increasingly welcome NMR as an allied technique in their structural analyses Indeed it may be that in the future crystal structures will be determined by simultaneously fitting diffraction patterns and NMR spectra This Handbook is organised into six sections The first contains an overview and some articles on fundamental NMR topics followed by a section concentrating on chemical shifts and one on coupling interactions The fourth section contains articles describing how NMR results relate to fundamental crystallography concepts and to diffraction methods The fifth section concerns specific aspects of structure such as hydrogen bonding Finally four articles in the sixth section give applications of NMR crystallography to structural biology organic pharmaceutical chemistry inorganic materials chemistry and geochemistry About EMR Handbooks eMagRes Handbooks The Encyclopedia of Magnetic Resonance up to 2012 and eMagRes from 2013 onward publish 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 EMR Handbooks eMagRes Handbooks on specific areas of NMR and MRI The chapters of each of these handbooks will comprise a carefully chosen selection of articles from eMagRes In consultation with the eMagRes Editorial Board the EMR Handbooks eMagRes Handbooks are coherently planned in advance by specially selected Editors and new articles are written together with

updates of some already existing articles 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 View other eMagRes publications [here](#)

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