

New Developments in NMR

Mikhail Elyashberg, Antony Williams and Kirill Blinov

Contemporary Computer-Assisted Approaches to Molecular Structure Elucidation



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Contemporary Computer Assisted Approaches To Molecular Structure Elucidation Rsc New Developments In Nmr

Giuseppe Pileio



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Contemporary Computer-Assisted Approaches to Molecular Structure Elucidation Mikhail E Elyashberg, Antony Williams, Kirill Blinov, 2015-11-09 Computer Assisted Structure Elucidation CASE systems are a combination of software algorithms and tools to support and enable chemists and spectroscopists engaged in the process of molecular structure elucidation via the analysis of spectroscopic data These expert systems dramatically reduce the time associated with structure elucidation and improve the reliability of the results Contemporary Computer Assisted Approaches to Molecular Structure Elucidation describes the principles on which these expert systems for spectroscopic structure elucidation are based and concisely explains the algorithmic concepts behind the programs The authors use their own personal experiences in the development of the Structure Elucidator StrucEluc CASE software system to discuss the present state of the art in computer assisted structure elucidation Scientists that are presently using CASE systems will be interested in the algorithms and modern approaches and for organizations that are currently using the StrucEluc platform the book is designed to help researchers understand the strategies behind CASE as well as details regarding the StrucEluc platform For scientists that have never used CASE systems they will now have access to all necessary information to understand CASE systems for mastering this new and very effective approach to structure elucidation The authors overall goal in writing this book is to produce the must read definitive text that will represent the results of decades of work to develop computer assisted structure elucidation software systems CASE systems are now powerful software tools commonly outperforming and correcting human interpretations of data This book will also provide an historical perspective of the work of the founding fathers of the technique and identify the challenges that have been overcome to produce modern CASE systems

Contemporary Computer-assisted Approaches to Molecular Structure Elucidation Mikhail Elyashberg, Antony Williams, Kirill Blinov, 2012 The first volume that describes the principles on which expert CASE systems for structure elucidation are based and concisely explains the algorithmic concepts behind the programs *Field-cycling NMR Relaxometry* Rainer Kimmich, 2018-10-16 Field cycling NMR relaxometry is evolving into a methodology of widespread interest Aimed at newcomers to the field and researchers in academia and industry this book will summarise the expertise of leading scientists in the area *Biophysics and Biochemistry of Cartilage by NMR and MRI* Yang Xia, Konstantin Momot, 2016-11-09 This unique book describes the latest information in the fundamental understanding of the biophysics and biochemistry of articular cartilage using the state of the art practices in NMR and MRI This is the first book of its kind written by physicists and chemists on this important tissue whose degradation contributes to osteoarthritis and related joint diseases Connecting the fundamental science with the clinical imaging applications the experts Editors provide an authoritative addition to the literature Ideal for practising physical scientists and radiologists with an interest in the

fundamental science as well as instrument manufacturers and clinical researchers working with articular cartilage

Advances in Biological Solid-State NMR Frances Separovic, Akira Naito, 2014-03-17 The complexity and heterogeneity of biological systems has posed an immense challenge in recent years. An increasingly important tool for obtaining molecular and atomic scale information on a range of large biological molecules and cellular components is solid state NMR. This technique can address fascinating problems in structural biology including the arrangement of supramolecular complexes and fibril formation in relation to molecular folding, misfolding and aggregation. Advances in Biological Solid State NMR brings the reader up to date with chapters from international leaders of this growing field covering the most recent developments in the methodology and applications of solid state NMR to studies of membrane interactions and molecular motions. A much needed discussion of membrane systems is detailed alongside important developments in in situ analysis. Topics include applications to biological membranes, membrane active peptides, membrane proteins, protein assemblies and in cell NMR. This exposition of an invaluable technique will interest those working in a range of related spectroscopic and biological fields. A basic introduction invites those interested to familiarise themselves with the basic mathematical and conceptual foundations of solid state NMR. A thorough and comprehensive discussion of this promising technique follows which is essential reading for those working or studying at postgraduate level in this exciting field. Mobile NMR and MRI

Mike Johns, Einar O. Fridjonsson, Sarah Vogt, Agnes Haber, 2015-10-27 This book will summarise recent hardware developments, highlight the challenges facing mobile and generally low field NMR and MRI and describe various emerging applications, some of which have commercial interest. **NMR-based Metabolomics** Hector C Keun, 2018-01-04 In the rapidly growing field of metabolomics, a comprehensive book describing the state of the art in the application of NMR spectroscopy will be a key title for practitioners. Providing a unique resource of background knowledge, resources, instrumental platforms and software, this book will introduce relevant theory to the researcher as well as serve as a practical guide detailing key experiments and data handling procedures. Information available on common sample types will be described together with reference to the latest web based resources available. Application specific considerations will be discussed for a wide range of research topics. Written by an expert team as a service to the metabolomics community, this book will appeal to NMR spectroscopists, analytical chemists and biochemists, especially those with an interest in medical applications. **Paramagnetism in Experimental Biomolecular NMR** Enrico Ravera, Giacomo Parigi, Claudio

Luchinat, 2018-08-06 Paramagnetic NMR is a growing technique that represents an increasingly important tool for the investigation of biomolecules. This book presents an update and overview of the paramagnetic NMR phenomena and effects as well as guidelines for practical implementation of state of the art experiments. All experiments are supported by a solid theoretical foundation. Areas mentioned are the development of solid state NMR, the use of paramagnetic tags providing information on the structure and mobility of the investigated systems and dynamic nuclear polarization to increase sensitivity.

Compiled by experts in the field this book has international appeal for researchers as well as students interested in magnetic resonance and structural biology who require experimental support and accessible information **Long-lived Nuclear**

Spin Order Giuseppe Pileio, 2020-04-07 The idea that a long lived form of spin order namely singlet order can be prepared from nuclear spin magnetisation first emerged in 2004 The unusual properties of singlet order its long lifetime and the fact that it is NMR silent but interconvertible into other forms of NMR active order make it a smart tag that can be used to store information for a long time or through distant space points It is not unexpected then that since its first appearance this idea has caught the attention of research groups interested in exploiting this form of order in different fields of research spanning from biology to materials science and from hyperpolarisation to quantum computing This first book on the subject gives a thorough description of the various aspects that affect the development of the topic and details the interdisciplinary applications The book starts with a section dedicated to the basic theories of long lived spin order and then proceeds with a description of the state of the art experimental techniques developed to manipulate singlet order It then concludes by covering the generalization of the concept of singlet order by introducing and discussing other forms of long lived spin order

NMR in Glycoscience and Glycotechnology Koichi Kato, Thomas Peters, 2017-05-17 This volume focuses on solution and solid state NMR of carbohydrates glycoproteins glyco technologies biomass and related topics Timely and useful it will appeal to researchers in the general field of structural biology biochemistry and biophysics molecular and cellular biology and material science **Contrast Agents for MRI** Valérie C Pierre, Matthew J Allen, 2017-11-09 As a practical reference

guide for designing and performing experiments this book focuses on the five most common classes of contrast agents for MRI namely gadolinium complexes chemical exchange saturation transfer agents iron oxide nanoparticles manganese complexes and fluorine contrast agents It describes how to characterize and evaluate them and for each class a description of the theory behind their mechanisms is discussed briefly to orient the new reader Detailed subchapters discuss the different physical chemistry methods used to characterize them in terms of their efficacy safety and in vivo behavior Important consideration is also given to the different physical properties that affect the performance of the contrast agents The editors and contributors are at the forefront of research in the field of MRI contrast agents and this unique cutting edge book is a timely addition to the literature in this area **Cross-relaxation and Cross-correlation Parameters in NMR**

Daniel Canet, 2017-10-20 This work will provide a detailed account of cross relaxation and cross correlation which would be timely and fill a gap in the present NMR literature for the analytical scientist [Fast NMR Data Acquisition](#) Mehdi

Mobli, Jeffrey C Hoch, 2017-05-18 Providing a definitive reference source on novel methods in NMR acquisition and processing this book will highlight similarities and differences between emerging approaches and focus on identifying which methods are best suited for different applications The highly qualified editors have conducted extensive research into the fundamentals of fast methods of data acquisition in NMR including applications of non Fourier methods of spectrum analysis

With contributions from additional distinguished experts in allied fields clear explanations are provided on methods that speed up NMR experiments using different ways to manipulate the nuclei in the sample modern methods for estimating the spectrum from the time domain response recorded during an NMR experiment and finally how the data is sampled Starting with a historical overview of Fourier Transformation and its role in modern NMR spectroscopy this volume will clarify and demystify this important emerging field for spectroscopists and analytical chemists in industry and academia Diffusion NMR of Confined Systems Rustem Valiullin, 2016-12-12 With the increasing role of porous solids in conventional and newly emerging technologies there is an urgent need for a deeper understanding of fluid behaviour confined to pore spaces of these materials especially with regard to their transport properties From its early years NMR has been recognized as a powerful experimental technique enabling direct access to this information In the last two decades the methodological development of different NMR techniques to assess dynamic properties of adsorbed ensembles has been progressed This book will report on these recent advances and look at new broader applications in engineering and medicine Having both academic and industrial relevance this unique reference will be for specialists working in the research areas and for advanced graduate and postgraduate studies who want information on the versatility of diffusion NMR Gas Phase NMR Karol Jackowski, Michał Jaszuński, 2016-02-09 This book covers the recent NMR studies with the application of gaseous molecules Among the comprehensively discussed aspects of the area it includes in particular new multinuclear experiments that deliver spectral parameters of isolated molecules and provide the most accurate values of nuclear magnetic shielding isotropic spin spin coupling and relaxation times advanced precise and correct theoretical descriptions of spectral parameters of molecules as well as the application of gas phase NMR measurements to chemical analysis and medicine The progress of research in these fields is enormous and has rapidly changed our knowledge and understanding of molecular parameters in NMR spectroscopy For example accurate studies of the shielding for isolated molecules allow the exact determination of nuclear magnetic dipole moments the calculated values of spectral parameters can be verified by precise gas phase NMR measurements and the application of hyperpolarized noble gases provides excellent MRI pictures of lungs Aimed at graduates and researchers in spectroscopy analytical chemistry and those researching the applications of NMR in medicine this book presents the connections between sophisticated experiments the theory of magnetic parameters and the exploration of new methods in practice **Optimizing NMR Methods for Structure Elucidation** Darcy C Burns, William F Reynolds, 2018-09-26 This book is aimed at informing organic chemists and natural products chemists on the use of NMR for structure elucidation to enable them to ensure they yield the most reliable possible data in the minimum possible time It covers the latest pulse sequences acquisition and processing methods practical areas not covered in most texts e g detailed consideration of the relative advantages and disadvantages of different pulse sequences choosing acquisition and processing parameters to get the best possible data in the least possible time pitfalls to avoid and how to minimize the risks of getting

wrong structures Useful in industrial pharma or research environments this reference book is for anyone involved with organic chemistry research and in particular natural products research requiring advice for getting the best results from the NMR facilities *Biophysics of Molecular Chaperones* Sebastian Hiller, Maili Liu, Lichun He, 2023-11-01 Molecular chaperones are critical to control protein quality in all living cells Understanding chaperone function at the atomic level and in particular its mode of interaction with client proteins is crucial to understanding the fundamental roles chaperones play in biology This book fills a gap in the literature by comprehensively summarizing and discussing new advanced experimental techniques for their analysis Providing a comprehensive overview of advanced biophysical methods for the characterization of molecular mechanisms of molecular chaperones the majority of the contributions are NMR methodology This is the method of choice for atomic resolution studies of such systems Additional notable biophysical approaches are considered to present all relevant current developments in exploring chaperone function and the transient and dynamic interactions with their client proteins The book is targeted at both current practitioners of structural biology and biophysical chemistry and scientists who are interested in entering the field It could be useful for graduate students as supplementary reading

Magnetic Resonance Technology Andrew G Webb, 2016-04-27 Magnetic resonance systems are used in almost every academic and industrial chemistry physics and biochemistry department as well as being one of the most important imaging modalities in clinical radiology The design of such systems has become increasingly sophisticated over the years Static magnetic fields increase continuously large scale arrays of receive elements are now ubiquitous in clinical MRI cryogenic technology has become commonplace in high resolution NMR and is expanding rapidly in preclinical MRI specialized high strength magnetic field gradients have been designed for studying the human connectome and the commercial advent of ultra high field human imaging has required new types of RF coils and static shim coils together with extensive electromagnetic simulations to ensure patient safety This book covers the hardware and engineering that constitutes a magnetic resonance system whether that be a high resolution liquid or solid state system for NMR spectroscopy a preclinical system for imaging animals or a clinical system used for human imaging Written by a team of experts in the field this book provides a comprehensive and instructional look at all aspects of current magnetic resonance technology as well as outlooks for future developments

Advanced Diffusion Encoding Methods in MRI Daniel Topgaard, 2020-08-06 The medical MRI community is by far the largest user of diffusion NMR techniques and this book captures the current surge of methods and provides a primary source to aid adoption in this field There is a trend to adapting the more advanced diffusion encoding sequences developed by NMR researchers within the fields of porous media chemical engineering and colloid science to medical research Recently published papers indicate great potential for improved diagnosis of the numerous pathological conditions associated with changes of tissue microstructure that are invisible to conventional diffusion MRI This book disseminates these recent developments to the wider community of MRI researchers and clinicians The chapters cover the

theoretical basis hardware and pulse sequences data analysis and validation and recent applications aimed at promoting further growth in the field This is a fast moving field and chapters are written by key MRI scientists that have contributed to the successful translation of the advanced diffusion NMR methods to the context of medical MRI from global locations

Hyperpolarized Xenon-129 Magnetic Resonance Thomas Meersmann, Eike Brunner, 2015-04-14 Providing the first comprehensive book on the current state of hyperpolarized Xenon 129 NMR and MRI this book is guaranteed to appeal to a wide range of scientists interested in this growing field It is intended to create synergy between the various communities working with this noble gas Covering all topics from the production of the hyperpolarized gas to its applications the editors have invited a leading team of experts to combine the physical chemistry within the various topics and across disciplines The scope will range from the fundamental aspects of optical pumping to practical aspects of hyperpolarizers and hp xenon handling The applications section will focus on hyperpolarized xenon 129 detected in the dissolved phase or micro porous media where the chemical shift of xenon 129 can be used as a diagnostic probe Appealing to researchers in the biomedical field and materials sciences this reference book will provide background reading and future looking material in one place

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