

***DYNAMIC  
NUCLEAR MAGNETIC  
RESONANCE  
SPECTROSCOPY***

*Edited by  
Lloyd M. Jackman and E. A. Cotton*

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# Dynamic Nuclear Magnetic Resonance Spectroscopy

**Vladimir K. Michaelis, Robert G.  
Griffin, Björn Corzilius, Shimon Vega**

## **Dynamic Nuclear Magnetic Resonance Spectroscopy:**

*Dynamic Nuclear Magnetic Resonance Spectroscopy* Lloyd Jackman, 2012-12-02 Dynamic Nuclear Magnetic Resonance Spectroscopy provides an overview of the state of knowledge in dynamic nuclear magnetic resonance DNMR spectroscopy. The early chapters describe the theoretical basis and practical techniques which have or will be used for extracting kinetic data from DNMR spectra. The subsequent chapters provide reviews of the many areas in which DNMR spectroscopy has been applied. Key topics covered include nuclear exchange processes, band shape analysis, application of nonselective pulsed NMR experiments, diffusion and chemical exchange, spin-spin relaxation time determination, rotation about single and double bonds in organic molecules and dynamic molecular processes in inorganic and organometallic compounds. Also discussed are studies on stereochemical nonrigidity in organometallic and metal carbonyl compounds, fluxional allyl complexes, carbonium ion rearrangements and proton transfer processes. It is hoped that this volume will provide a literature guide, source book and progress report which will be helpful to all those who will continue or will begin work in this field. **Dynamic NMR**

**Spectroscopy**, 2012-12-06 Since the first successful NMR experiments in 1946 it was well appreciated that dynamic processes play an important role in the NMR spectroscopy of bulk matter. 1 Early theories on the dependence of the relaxation parameters  $T_1$  and  $T_2$  on the motions of nuclear spins were successful in explaining the dipolar broadening of the NMR signal in solids and the motional narrowing in liquids. 2 With the discovery of chemical shifts and spin-spin couplings another type of dynamical process affecting the NMR line shape became apparent: the chemical exchange. As a consequence dynamical NMR studies split into two groups differing not only in the dynamical topics but also in the method of investigation: physical studies of the motion of spins in liquids and solids by measurement of the relaxation times of single resonances and on the other hand chemical studies based on band shape analysis of NMR spectra recorded under steady state conditions. The two fields of research lost some of their basic differences with the development of the Fourier transform NMR method. 3

which allows the measurement of relaxation times of different resonances at the same time, i.e. the study of differential motional behavior of different parts of molecules thus providing a new tool in conformational analyses. For example information can be obtained by this method on the relative importance of overall motions and internal motions. 4 Dynamic Nuclear Magnetic Resonance Spectroscopy

Lloyd M. Jackman, F. A. Cotton, 1977 Handbook of High Field Dynamic

Nuclear Polarization Vladimir K. Michaelis, Robert G. Griffin, Björn Corzilius, Shimon Vega, 2019-12-12 Addresses Dynamic Nuclear Polarization DNP as a technique for sensitivity enhancement in solid state NMR spectroscopy. This comprehensive handbook is a compendium of the current state of the art of high field Dynamic Nuclear Polarization from long proven early developments up to today's hot topics. It covers all the relevant subjects that have made a direct or indirect contribution toward advancing this field and focuses on topics such as the theory behind the effects seen within DNP instrumentation required for carrying out DNP and specific applications of DNP including protein monitoring, catalysis, nanoparticles.

biological and clinical studies Development and application of techniques that have indirectly contributed to advancing MAS DNP NMR such as DNP experiments on static solids within microwave resonant structures and high field EPR are also examined Handbook of High Field Dynamic Nuclear Polarization is presented in three sections Theoretical Aspects DNP Development instrumentation radical sample and DNP NMR Applications The first section offers chapters on solid and cross effect DNP thermal mixing Overhauser and dissolution DNP The second looks at microwave technology gyrotron and IOE homebuilt and commercial DNP spectrometers and glassing vs solvent free DNP The final section provides information on amyloid membrane and nanocrystalline proteins metals and surface enhanced DNP pharmaceuticals nanoparticles and much more Covers one of the biggest developing fields in magnetic resonance Relevant to students academics and industry within the physical materials medical and biochemical sciences An excellent starting point and point of reference for researchers in the field Edited by a widely respected team with contributions from key researchers in the NMR community Part of the eMagRes Handbook Series Handbook of High Field Dynamic Nuclear Polarization is an ideal reference for all researchers and graduate students involved in this complex interdisciplinary field About eMagRes Handbooks eMagRes 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 eMagRes Handbooks on specific areas of NMR and MRI The chapters of each of these handbooks will comprise a carefully chosen selection of eMagRes articles In consultation with the eMagRes Editorial Board the eMagRes Handbooks are coherently planned in advance by specially selected Editors and new articles are written 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](http://www.wileyonlinelibrary.com/ref/eMagRes)

Progress in Nuclear Magnetic Resonance Spectroscopy. ,1973      **Dynamic NMR Spectroscopy** J. Sandström,1982

DYNAMIC NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY. FA COTTON (ED.),1975      Studies in Dynamic

Nuclear Magnetic Resonance Spectroscopy Robert Cort Hadden,      *Quantitative Determination of Chemical Processes by Dynamic Nuclear Polarization Enhanced Nuclear Magnetic Resonance Spectroscopy* Haifeng Zeng,2012 Dissolution dynamic nuclear polarization DNP provides several orders of magnitude of NMR signal enhancement by converting the much larger electron spin polarization to nuclear spin polarization Polarization occurs at low temperature 1-4K and is followed by quickly dissolving the sample for room temperature NMR detection DNP is generally applicable to almost any small molecules and can polarize various nuclei including  $^1\text{H}$   $^{19}\text{F}$  and  $^{13}\text{C}$  The large signal from DNP enhancement reduces the limit of detection to micromolar or sub micromolar concentration in a single scan Since DNP enhancement often provides the only source for the observable signal it enables tracking of the polarization flow Therefore DNP is ideal for studying chemical processes Here

quantitative tools are developed to separate kinetics and spin relaxation as well as to obtain structural information from these measurements. Techniques needed for analyzing DNP polarized sample are different from those used in conventional NMR because a large yet non renewable hyperpolarization is available. Using small flip angle pulse excitation the hyperpolarization can still be divided into multiple scans. Based on this principle a scheme is presented that allows reconstruction of indirect spectral dimensions similarly to conventional 2D NMR. Additionally small flip angle pulses can be used to obtain a succession of scans separated in time. A model describing the combined effects of the evolution of a chemical process and of spin lattice relaxation is shown. Applied to a Diels Alder reaction it permitted measuring kinetics along with the effects of auto and cross relaxation. DNP polarization of small molecules also shows significant promise for studying protein ligand interaction. The binding of fluorinated ligands to the protease trypsin was studied through the observation of various NMR parameter changes such as line width, signal intensity and chemical shift of the ligands. Intermolecular polarization transfer from hyperpolarized ligand to protein can further provide information about the binding pocket of the protein. As an alternative to direct observation of protein signal a model is presented to describe a two step intermolecular polarization transfer between competitively binding ligands mediated through the common binding pocket of the protein. The solutions of this model relate the evolution of signal intensities to the intermolecular cross relaxation rates which depend on individual distances in the binding epitope. In summary DNP provides incomparable sensitivity, speed and selectivity to NMR. Quantitative models such as those discussed here enable taking full advantage of these benefits for the study of chemical processes.

### **Chemically Induced Dynamic Nuclear and Electron Polarizations-CIDNP and CIDEP**

C. Richard, P. Granger, 2012-12-06. Anomalous electron spin state populations in the Electron Paramagnetic Resonance (EPR) spectra of radicals formed during radiolysis experiments were observed in 1963 by FESSENDEN and SCHULER<sup>170a</sup>. This phenomenon did not receive much attention at the time. In 1967 BARGON FISCHER and JOHNSEN<sup>5</sup> and independently WARD and LAWLER<sup>7,8</sup> reported a similar phenomenon for Nuclear Magnetic Resonance (NMR) spectra taken during radical reactions, emission or enhanced absorption or both. The earliest attempts to explain this new NMR phenomenon treated these effects in a way similar to that of Dynamic Nuclear Polarization (DNP) or the Overhauser effect. Although the polarization has a completely different origin, DNP gave its name to this effect: Chemically Induced Dynamic Nuclear Polarization (CIDNP). The name Chemically Induced Dynamic Electron Polarization (CIDEP) was introduced later by analogy with CIDNP. After the initial publications, all the new data demonstrated that the first theory could not be correct. In 1969 a new theory was proposed by CLOSS<sup>18</sup> and independently by KAPTEIN and OOSTERHOFF<sup>23</sup> and called the radical pair theory. This mechanism was proposed to account for the observations of polarization in both NMR and EPR. The radical pair theory is based on weak interactions in a pair of radicals; the strength of interaction between the electronic states of the radicals depends in particular on the nuclear spin states.

*Dynamic Hyperpolarized Nuclear Magnetic Resonance* Thomas Jue, Dirk Mayer, 2021-05-21

This is the first book in the series to focus on dynamic hyperpolarized nuclear magnetic resonance a burgeoning topic in biophysics The volume follows the format and style of the Handbook of Modern Biophysics series and expands on topics already discussed in previous volumes It builds a theoretical and experimental framework for students and researchers who wish to investigate the biophysics and biomedical application of dynamic hyperpolarized NMR All contributors are internationally recognized experts lead the dynamic hyperpolarized NMR field and have first hand knowledge of the chapter material The book covers the following topics Hyperpolarization by dissolution Dynamic Nuclear Polarization Design considerations for implementing a hyperpolarizer Chemical Shift Imaging with Dynamic Hyperpolarized NMR Signal Sampling Strategies in Dynamic Hyperpolarized NMR Kinetic Modeling of Enzymatic Reactions in Analyzing Hyperpolarized NMR Data Using Hyperpolarized NMR to Understand Biochemistry from Cells to Humans Innovating Metabolic Biomarkers for Hyperpolarized NMR New Insights into Metabolic Regulation from Hyperpolarized  $^{13}\text{C}$  MRS MRI Studies Novel Views on Heart Function from Dynamic Hyperpolarized NMR Insights on Lactate Metabolism in Skeletal Muscle based on  $^{13}\text{C}$  Dynamic Nuclear Polarization Studies About the Editors Dirk Mayer is Professor of Diagnostic Radiology and Nuclear Medicine at the University of Maryland and is the Director of Metabolic Imaging He is a recognized expert on dynamic nuclear polarization DNP MRI based imaging techniques and has optimized acquisition and reconstruction techniques has constructed kinetic modeling for quantitative analysis and has developing new probes Thomas Jue is Professor of Biochemistry and Molecular Medicine at the University of California Davis He is an internationally recognized expert in developing and applying magnetic resonance techniques to study animal as well as human physiology in vivo He served as a Chair of the Biophysics Graduate Group Program at UC Davis where he started to redesign a graduate curriculum that balances physical science mathematics formalism and biomedical perspective in order to promote interest at the interface of physical science engineering mathematics biology and medicine The Handbook of Modern Biophysics represents an aspect of that effort

**Nuclear Magnetic Resonance Spectroscopy** John Henry Nelson, 2003 This is the only how to volume that investigates the spectroscopy of a variety of nuclides other than H and C in depth It contains extensive reference material and numerous problems most of which include real spectra It is written to provide users with the knowledge necessary to choose the most appropriate experiment to obtain the best quality spectra with the ability to fully interpret the data The book covers basic theory of NMR spectroscopy spectrum measurement the chemical shift and examples for selected nuclei symmetry and NMR spectroscopy spin spin coupling and NMR spin systems typical magnitude of selected coupling constants nuclear spin relaxation the nuclear overhauser effect editing C NMR spectra two dimensional NMR spectroscopy dynamic NMR spectroscopy lanthanide shift reagents LSR NMR of solids For NMR spectroscopists and analytical chemists *Nuclear Magnetic Resonance Spectroscopy* Pál Sohár, 1983 V 1 Theory of nuclear magnetic resonance spectroscopy NMR spectrometers recording techniques measuring methods v 2 Proton resonance spectroscopy The resonance spectra of nuclei

other than hydrogen v 3 Structure determination problems      **Annual Reports on NMR Spectroscopy** ,1999-10-04 These indexes are valuable volumes in the serial bringing together what has been published over the past 38 volumes They include a preface by the editor of the series an author index a subject index a cumulative list of chapter titles and listings of contents by volume      Conformational Properties of Unsaturated Medium-rings Dynamic Nuclear Magnetic Resonance Spectroscopy and Iterative Force-field Calculations Issa Yavari,1977      *Dynamic Nuclear Magnetic Resonance Spectroscopy of Diazoesters* Sarah M. Cureton,1997      *Chemically Induced Dynamic Nuclear Polarization* ,1973\*      **Conformational Properties of Unsaturated Medium-rings, Dynamic Nuclear Magnetic Resonance Spectroscopy, and Iterative Force-field Calculations** Mehran Ghiaci,1979      *The Chemistry of Hyperpolarized Magnetic Resonance Probes* Eul Hyun Suh,Zoltan Kovacs,2024-06-01 The Chemistry of Hyperpolarized Magnetic Resonance Probes Volume Seven focuses on the chemical aspects of hyperpolarized NMR MRI technology with synthesis and characterizations of labeled compounds discussed from a practical point of view A brief overview of the various hyperpolarization techniques are given with the optimization of hyperpolarization conditions and the determination of critical parameters such as polarization level and T1 relaxation values described A practical guide on the in vivo applications of hyperpolarized compounds in small animals is also included Helps readers understand the structural features that determine the properties of HP probes such as chemical shift and relaxation times Aids readers in selecting stable isotope labeled probes for hyperpolarized NMR MRI applications Teachers readers how to use the most appropriate synthetic methodology for the labeled probes Covers how to find the most suitable polarization technique DNP PHIP etc for the probe      **Carbon-13 Nuclear Magnetic Resonance Spectroscopy** George C. Levy,Robert L. Lichter,Gordon L. Nelson,1992

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