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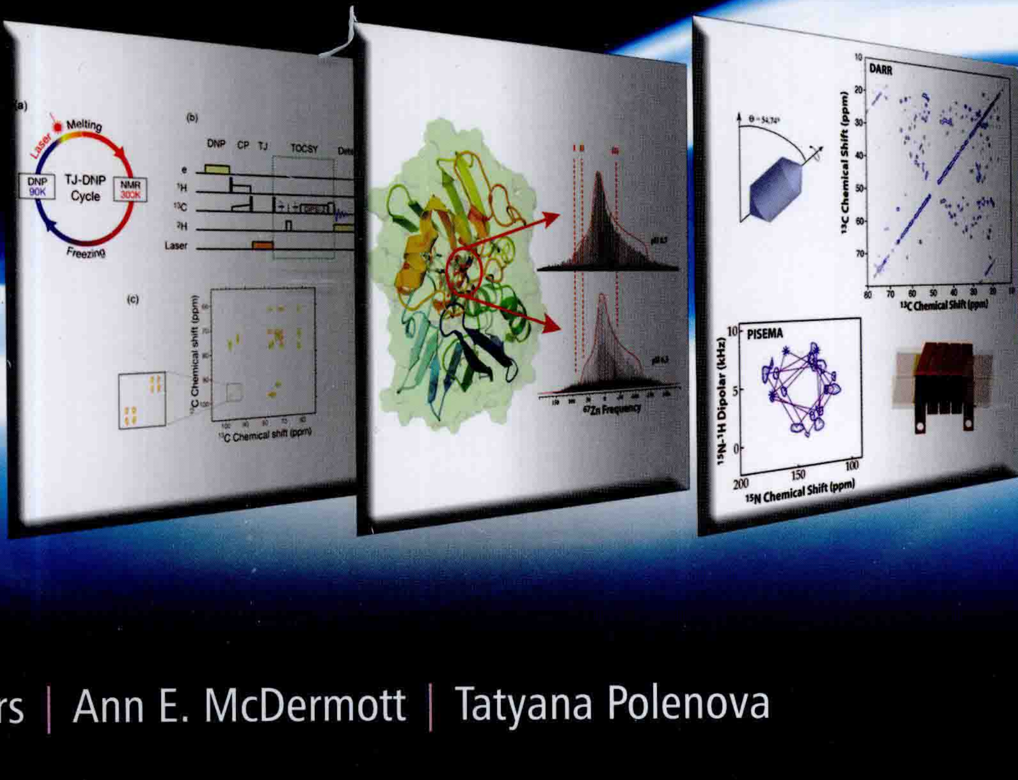
SOLID-STATE NMR STUDIES OF BIOPOLYMERS



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EMR

Solid-State NMR Studies of Biopolymers

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PS	Phosphorothioate
PS1	Photosystem I
PS2	Photosystem II
2Q	Double Quantum
2Q-HORROR	Double-Quantum Homonuclear Rotary Resonance
2QF-COSY	Double-Quantum-Filtered Correlation Spectroscopy
QCPMG	Quadrupole Carr–Purcell–Meiboom–Gill
QE	Quadrupolar Echo
QM	Quantum Mechanical
QM/MM	Quantum Mechanics/Molecular Mechanics
RC	Reaction Center
Rd	Rubredoxin
RDC	Residual Dipolar Coupling
REDOR	Rotational Echo Double Resonance
RF	Radio Frequency
RFDR	Radio-Frequency Driven Recoupling
RMSD	Root Mean Square Deviation
ROCSA	Recoupling of Chemical Shift Anisotropy
Rubisco	Ribulose-1,5-Bisphosphate Carboxylase/Oxygenase
RR	Rotational Resonance
RRTR	Rotational Resonance in the Tilted Rotating Frame
SB	Schiff Base
SCT	Semiconstant-Time
SDR	Stochastic Dipolar Recoupling
SE	Solid Effect
SEASHORE	Shift Evolution Assisted Selective HOmonuclear REcoupling
SEDRA	Simple Excitation for the Dephasing of Rotational Echo Amplitudes
SEMA	Spin Exchange at the Magic Angle
SERCA	Sarcoplasmic Reticulum Calcium ATPase
SF	Selectivity Filter
SLF	Separated Local Field
S3P	Shikimate-3-Phosphate
SPI-R^3	Simultaneous Phase Inversion Rotary Resonance
SQ	Single Quantum
SSHBs	Short, Strong Hydrogen Bonds
SSNMR	Solid-State Nuclear Magnetic Resonance
SSS	Space-Spin Selection
STR	Second Tilted Rotating
TAR	Transactivation Response Element
TCL	Tool Command Language
TEDOR	Transferred Echo Double Resonance
TEDOR-REDOR	Transferred Echo Double Resonance-Rotational Echo Double Resonance
TIM	Triosephosphate Isomerase
T-MREV	MREV-8
TJ	Temperature-Jump
TM	Thermal Mixing
TM	Transmembrane
TMS	Tetramethylsilane
TOBSY	Through Bond Spectroscopy
TOCSY	Total Correlation Spectroscopy
TOTAPOL	1-(TEMPO-4-Oxy)-3-(TEMPO-4-Amino)-Propan-2-Ol
TPPM	Two-Pulse Phase Modulation
TRNOE	Transferred Nuclear Overhauser Effect
UC	Uniform-Sign Cross-Peak
UC2QF-COSY	Uniform-Sign Cross-Peak Double-Quantum-Filtered Correlation Spectroscopy
UDG	Uracil DNA Glycosylase
VACP	Variable Amplitude Cross Polarization
VAS	Variable Angle Spinning
VEDs	Vacuum Electronic Devices
VT	Variable Temperature
WALTZ	Wonderful Alternating Phase Technique for Zero Residual Splittings
WT	Wild Type
ZQ	Zero Quantum

Solid-State NMR Studies of Biopolymers

EMR Handbooks

Based on the *Encyclopedia of Magnetic Resonance* (EMR), this monograph series focuses on hot topics and major developments in modern magnetic resonance and its many applications. Each volume in the series will have a specific focus in either general NMR or MRI, with coverage of applications in the key scientific disciplines of physics, chemistry, biology or medicine. All the material published in this series, plus additional content, will be available in the online version of EMR, although in a slightly different format.

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Encyclopedia of Magnetic Resonance

Edited by Robin K. Harris, Roderick E. Wasylishen, Edwin D. Becker, John R. Griffiths, Vivian S. Lee, Ian R. Young, Ann E. McDermott, Tatyana Polenova, James W. Emsley, George A. Gray, Gareth A. Morris, Melinda J. Duer and Bernard C. Gerstein.

The *Encyclopedia of Magnetic Resonance* (EMR) is based on the original printed *Encyclopedia of Nuclear Magnetic Resonance*, which was first published in 1996 with an update volume added in 2000. EMR was launched online in 2007 with all the material that had previously appeared in print. New updates have since been and will be added on a regular basis throughout the year to keep the content up to date with current developments. Nuclear was dropped from the title to reflect the increasing prominence of MRI and other medical applications. This allows the editors to expand beyond the traditional borders of NMR to MRI and MRS, as well as to EPR and other modalities. EMR covers all aspects of magnetic resonance, with articles on the fundamental principles, the techniques and their applications in all areas of physics, chemistry, biology and medicine for both general NMR and MRI. Additionally, articles on the history of the subject are included.

For more information see: http://www.mrw.interscience.wiley.com/emr

Encyclopedia of Magnetic Resonance

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Series Preface

The *Encyclopedia of Nuclear Magnetic Resonance* was published in eight volumes in 1996, in part to celebrate the fiftieth anniversary of the first publications in NMR in January 1946. Volume 1 contains an historical overview and ca. 200 short personal articles by prominent NMR practitioners, while the remaining seven volumes comprise ca. 500 articles on a wide variety of topics in NMR (including MRI). Two "spin-off" volumes incorporating the articles on MRI and MRS (together with some new ones) were published in 2000 and a ninth volume was brought out in 2002. In 2006, the decision was taken to publish all the articles electronically (i.e. on the World Wide Web) and this was carried out in 2007. Since then, new articles have been placed on the web every three months and a number of the original articles have been updated. This process is continuing. The overall title has been changed to the *Encyclopedia of Magnetic Resonance* to allow for future articles on EPR and to accommodate the sensitivities of medical applications.

The existence of this large number of articles, written by experts in various fields, is enabling a new concept to be implemented, namely the publication of a series of printed handbooks on specific areas of NMR and MRI. The chapters of each of these handbooks will comprise a carefully chosen selection of Encyclopedia articles relevant to the area in question. In consultation with the Editorial Board, the handbooks are coherently planned in advance by specially selected editors. New articles are written and existing articles are updated to give appropriate complete coverage of the total area. The handbooks are intended to be of value and interest to research students, postdoctoral fellows, and other researchers learning about the topic in question and undertaking relevant experiments, whether in academia or industry.

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Volume Preface

The purpose of this handbook is to provide a comprehensive introduction to modern biological solid-state NMR spectroscopy for students and for the general audience of scientists interested in entering the field. There has hitherto been no single volume that both covers the fundamentals in solid-state NMR theory and hardware and provides examples of contemporary applications. This handbook represents our efforts to remedy the growing need for such a treatment.

The selection of chapters is intended to give the interested reader a flavor of the richness of this rapidly developing field. The diverse nature of the experimental approaches and sample conditions, together with the high information content arising from the sensitivity of the various spin interactions to the environment and from the accumulated knowledge in the field – allowing a practising solid-state NMR spectroscopist to measure those interactions, extract the relevant physical observables and relate them to the molecular framework (i.e., geometry, electronic structure, molecular motions) through the accumulated empirical knowledge or through quantum chemical calculations – permits a wide range of biological systems to be studied at atomic-level detail.

Traditionally, solid-state NMR experiments in biological systems have focused on probing a single or a very small number of isotopically labeled sites; however, recent breakthroughs in hardware technology and pulse sequence developments have permitted high-resolution studies of uniformly and extensively labeled proteins and other biopolymers. A decade ago, the first reports emerged demonstrating that resonance assignments of uniformly isotopically enriched microcrystalline proteins are feasible using 2D and 3D magic-angle spinning spectroscopy, while subsequent investigations showed that 3D protein structures can be determined on the basis of distance and torsion angle constraints acquired in solid-state NMR experiments.

Since these initial studies, the field has experienced a spectacular growth in the number of solid-state NMR-based protein structures deposited in the Protein Data Bank, including studies of large proteins, membrane proteins, and protein assemblies that had previously been intractable using any structural biology method. Recent demonstrations that protein structures can be determined on the basis of isotropic chemical shifts alone have opened a vista of exciting opportunities for researchers entering the field.

The handbook starts with an introduction to fundamental concepts in spin physics. This is followed by a discussion of modern solid-state NMR experiments and the corresponding theoretical framework for extracting structural and dynamics information in biological systems, including recoupling and coherence transfer techniques; a review of quantum mechanical calculations of NMR spectroscopic observables follows. Computational approaches to structure calculations are presented. Discussion of the experiments for measurements of molecular motions and their interpretation is included. Modern solid-state NMR probe hardware is also described. Finally, a series of chapters on applications of contemporary solid-state NMR methods to a broad range of biological systems is presented.

We note that the field of biological solid-state NMR spectroscopy is so diverse and developing so rapidly that we have not been able to cover all topics in depth or indeed in some cases, at all. For example, some of the emerging methodologies (e.g., signal enhancement protocols through CIDNP and half-integer quadrupolar nuclei) are introduced briefly, and the interested reader is encouraged to seek additional chapters on these important topics in the *Encyclopedia of Magnetic Resonance*. Furthermore, technical advances in the field are unfolding even as we are preparing this handbook for press, and these will be included in future editions. It is, we feel, an exciting time for a new generation of researchers to enter the field of biological solid-state NMR spectroscopy.

We are very grateful to our colleagues—the authors of the chapters, who have contributed their time and expertise to this handbook. We hope that it will become a useful resource for a broad readership of scientists interested in solid-state NMR spectroscopy.

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