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Course

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The content of this volume has
been added to eMagRes

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(formerly Encyclopedia of
Magnetic Resonance) - the
ultimate online resource for NMR
and MRI. Over the past 20 years
technical developments in
superconducting magnet
technology and instrumentation

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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

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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

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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,

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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

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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

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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

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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,

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semiconductors and high-
temperature superconductors.

About EMR Handbooks /
eMagRes Handbooks The
Encyclopedia of Magnetic
Resonance (up to 2012) and
eMagRes (from 2013 onward)

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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

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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

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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

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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

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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

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The Second Edition of the
Encyclopedia of Spectroscopy
and Spectrometry pulls key

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techniques and new insights for comprehensive coverage of the field. The content is available in print and online via ScienceDirect, the latter of which offers optimal flexibility, accessibility, and usability

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other work gives analytical and
physical (bio)chemists such
unprecedented access to the
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SPEC-2 maintains the "authoritative, balanced coverage" of the original work while also breaking new ground in spectroscopic research. Incorporates more than 150 color figures, 5,000 references, and

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300 articles (30% of which are new), for a thorough examination of the field Highlights new research and promotes innovation in applied areas ranging from food science and forensics to biomedicine and

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health Features a new co-editor:
David Koppenaal of Pacific
Northwest National Laboratory,
Washington, USA, whose work
in atomic mass spectrometry has
been recognized internationally
This book is the perfect link for

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learning how to perform the experiments after only having studied theory. In eight chapters more than 50 essential NMR experiments are described in detail. Special focus is put on the organic set of NMR spectra (^1H ,

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¹³C-APT, COSY, NOESY, HSQC and HMBC). Different chapters deal with advanced organic NMR, selective methods, heteronuclear NMR, relaxation and diffusion measurements, organic applications and

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maintenance. Every experiment has a section providing the reader with the purpose and scope of the specific experiment. Every experiment is concluded with the spectrum as it is obtained under the conditions

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described. Questions and comments enable the reader to check their understanding. The authors are very experienced and the whole book is in full color, which enhances the reading experience and makes

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the spectra and other figures easier to understand. This book is strongly recommended for all students and researchers who are involved in the structural elucidation of chemical compounds both in practical

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education and in pursuing research, in particular if they handle an NMR spectrometer. This volume will focus on a theme - NMR applications in industry and providing a comprehensive yet critical review

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of the current literature from various industries.

This book intends to be an easy and concise introduction to the field of nuclear magnetic resonance or NMR, which has revolutionized life sciences in the

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last twenty years. A significant part of the progress observed in scientific areas like Chemistry, Biology or Medicine can be ascribed to the development experienced by NMR in recent times. Many of the books

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currently available on NMR deal with the theoretical basis and some of its main applications, but they generally demand a strong background in Physics and Mathematics for a full understanding. This book is

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aimed to a wide scientific audience, trying to introduce NMR by making all possible effort to remove, without losing any formality and rigor, most of the theoretical jargon that is present in other NMR books.

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Furthermore, illustrations are provided that show all the basic concepts using a naive vector formalism, or using a simplified approach to the particular NMR-technique described. The intention has been to show

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simply the foundations and main concepts of NMR, rather than seeking thorough mathematical expressions.

The derivation of structural information from spectroscopic data is now an integral part of

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organic chemistry courses at all Universities. Over recent years, a number of powerful two-dimensional NMR techniques (e.g. HSQC, HMBC, TOCSY, COSY and NOESY) have been developed and these have vastly

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expanded the amount of structural information that can be obtained by NMR spectroscopy. Improvements in NMR instrumentation now mean that 2D NMR spectra are routinely (and sometimes automatically)

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acquired during the identification and characterisation of organic compounds. Organic Structures from 2D NMR Spectra is a carefully chosen set of more than 60 structural problems employing 2D-NMR spectroscopy. The

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problems are graded to develop and consolidate a student's understanding of 2D NMR spectroscopy. There are many easy problems at the beginning of the collection, to build confidence and demonstrate the

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basic principles from which structural information can be extracted using 2D NMR. The accompanying text is very descriptive and focussed on explaining the underlying theory at the most appropriate level to

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sufficiently tackle the problems.
Organic Structures from 2D NMR
Spectra Is a graded series of
about 60 problems in 2D NMR
spectroscopy that assumes a
basic knowledge of organic
chemistry and a basic knowledge

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of one-dimensional NMR
spectroscopy Incorporates the
basic theory behind 2D NMR and
those common 2D NMR
experiments that have proved
most useful in solving structural
problems in organic chemistry

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Focuses on the most common 2D NMR techniques – including COSY, NOESY, HMBC, TOCSY, CH-Correlation and multiplicity-edited C-H Correlation.

Incorporates several examples containing the heteronuclei ^{31}P ,

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¹⁵N and ¹⁹F Organic Structures from 2D NMR Spectra is a logical follow-on from the highly successful “Organic Structures from Spectra” which is now in its fifth edition. The book will be invaluable for students of

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Chemistry, Pharmacy,
Biochemistry and those taking
courses in Organic Chemistry.
Also available: Instructors Guide
and Solutions Manual to Organic
Structures from 2D NMR Spectra
This work-book will guide you

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safely, in step-by-step descriptions, through every detail of the NMR experiments within, beginning with 1D routine experiments and ending with a series of advanced 3D experiments on a protein: .

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Which experiment can best yield the desired information? · How must the chosen experiment be performed? · How does one read the required information from the spectrum? · How does this particular pulse sequence work?

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• Which other experiments give similar information? This third edition of the book, following its two highly successful predecessors, has been revised and expanded to 206 experiments. They are organized

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in 15 chapters, covering test procedures and routine spectra, variable temperature measurements, the use of auxiliary reagents, 1D multipulse experiments, spectra of heteronuclides, and the

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application of selective pulses. The second and third dimensions are introduced using pulsed field gradients, and experiments on solid state materials are described. A key part describes 3D experiments on the protein

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ubiquitin with 76 amino acids.

What is new in this third edition?

1. 24 new experiments have been inserted into the 14 chapters that were in the 2nd edition, e.g., alpha/beta-SELINCOR-TOCSY, WET,

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DOSY, ct-COSY, HMSC, HSQC with adiabatic pulses, HETLOC. J-resolved HMBC, (1,1)- and (1,n)-ADEQUATE, STD, REDOR, and HR-MAS. 2. 20 new protein NMR experiments have been specially devised and

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are collected in the newly added Chapter 15, ProteinNMR, for which one needs a special model sample: fully ^{13}C - and ^{15}N -labeled human ubiquitin.

Techniques used include the constant time principle, the PEP

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method, filters, gradient selection, and the echo/anti-echo procedure. The guide has been written by experts in this field, following the principle of learning by doing: all the experiments have been specially performed

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for this book, exactly as described and shown in the spectra that are reproduced. Being a reference source and work-book for the NMR laboratory as well as a textbook, it is a must for every scientist

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working with NMR, as well as for
students preparing for their
laboratory courses

A blend of theory and practical
advice, Modern NMR

Techniques for Synthetic

Chemistry illustrates how NMR

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spectroscopy can be used to determine the abundance, size, shape, and function of organic molecules. It provides you with a description the NMR technique used (more pictorial than mathematical), indicating the

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most common pulse sequences,
some practical information as
appropriate, followed by
illustrative examples. This format
is followed for each chapter so
you can skip the more theoretical
details if the practical aspects

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are what interest you. Following a discussion of basic parameters, the book describes the utility of NMR in detecting and quantifying dynamic processes, with particular emphasis on the usefulness of

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saturation-transfer (STD) techniques. It details pulsed-field gradient approaches to diffusion measurement, diffusion models, and approaches to 'inorganic' nuclei detection, important as many synthetic pathways to new

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organics involve heavier elements. The text concludes with coverage of applications of NMR to the analysis of complex mixtures, natural products, carbohydrates, and nucleic acids—all areas of activity for

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researchers working at the chemistry-life sciences interface. The book's unique format provides some theoretical insight into the NMR technique used, indicating the most common pulse sequences. The book

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draws upon several NMR methods that are resurging or currently hot in the field and indicates the specific pulse sequence used by various spectrometer manufacturers for each technique. It examines the

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analysis of complex mixtures, a feature not found in most books on this topic.

[Principles and Practice](#)

[50 and More Essential NMR](#)

[Experiments](#)

[Isolation and Structure](#)

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[Elucidation of Natural Products](#)

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[A Practitioner's Guide](#)

[Drug-DNA Interactions](#)

[NMR for Chemists and Biologists](#)

[Chemical Analysis of Food](#)

[Basic One- and Two-](#)

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[Dimensional NMR Spectroscopy](#)
[Encyclopedia of Spectroscopy](#)
[and Spectrometry](#)
[Raman Spectroscopy](#)

*Presents an introduction to
modern NMR methods at a level
suited to organic and inorganic*

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chemists engaged in the solution of structural and mechanistic problems. The book assumes familiarity only with the simple use of proton and carbon spectra as sources of structural information and describes the

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advantages of pulse and Fourier transform spectroscopy which form the basis of all modern NMR experiments. Discussion of key experiments is illustrated by numerous examples of the solutions to real problems. The

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emphasis throughout is on the practical side of NMR and the book will be of great use to chemists engaged in both academic and industrial research who wish to realise the full possibilities of the new wave

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NMR.

*PRINCIPLES OF
INSTRUMENTAL ANALYSIS is
the standard for courses on the
principles and applications of
modern analytical instruments. In
the 7th edition, authors Skoog,*

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Holler, and Crouch infuse their popular text with updated techniques and several new Instrumental Analysis in Action case studies. Updated material enhances the book's proven approach, which places an

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emphasis on the fundamental principles of operation for each type of instrument, its optimal area of application, its sensitivity, its precision, and its limitations. The text also introduces students to elementary analog and digital

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*electronics, computers, and the
treatment of analytical data.*

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description or the product text
may not be available in the
ebook version.*

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The derivation of structural information from spectroscopic data is now an integral part of organic chemistry courses at all Universities. A critical part of any such course is a suitable set of problems to develop the

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student's understanding of how structures are determined from spectra. Organic Structures from Spectra, Fifth Edition is a carefully chosen set of more than 280 structural problems employing the major modern

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spectroscopic techniques, a selection of 27 problems using 2D-NMR spectroscopy, more than 20 problems specifically dealing with the interpretation of spin-spin coupling in proton NMR spectra and 8 problems based

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on the quantitative analysis of mixtures using proton and carbon NMR spectroscopy. All of the problems are graded to develop and consolidate the student's understanding of organic spectroscopy. The

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*accompanying text is descriptive
and only explains the underlying
theory at a level which is
sufficient to tackle the problems.
The text includes condensed
tables of characteristic spectral
properties covering the*

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*frequently encountered
functional groups. The examples
themselves have been selected
to include all important common
structural features found in
organic compounds and to
emphasise connectivity*

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*arguments. Many of the
compounds were synthesised
specifically for this purpose.
There are many more easy
problems, to build confidence
and demonstrate basic
principles, than in other*

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collections. The fifth edition of this popular textbook: • includes more than 250 new spectra and more than 25 completely new problems; • now incorporates an expanded suite of new problems dealing with the analysis of 2D

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*NMR spectra (COSY, C H
Correlation spectroscopy,
HMBC, NOESY and TOCSY); •
has been expanded and updated
to reflect the new developments
in NMR and to retire older
techniques that are no longer in*

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common use; • provides a set of problems dealing specifically with the quantitative analysis of mixtures using NMR spectroscopy; • features proton NMR spectra obtained at 200, 400 and 600 MHz and ¹³C NMR

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spectra include DEPT experiments as well as proton-coupled experiments; • contains 6 problems in the style of the experimental section of a research paper and two examples of fully worked

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*solutions. Organic Structures
from Spectra, Fifth Edition will
prove invaluable for students of
Chemistry, Pharmacy and
Biochemistry taking a first course
in Organic Chemistry. Contents
Preface Introduction Ultraviolet*

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Spectroscopy Infrared

Spectroscopy Mass

Spectrometry Nuclear Magnetic

Resonance Spectroscopy

2DNMR Problems Index

Reviews from earlier editions

"Your book is becoming one of

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the “go to” books for teaching structure determination here in the States. Great work!” “...I would definitely state that this book is the most useful aid to basic organic spectroscopy teaching in existence and I would

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*strongly recommend every
instructor in this area to use it
either as a source of examples
or as a class textbook”.*

*Magnetic Resonance in
Chemistry “Over the past year I
have trained many students*

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using problems in your book - they initially find it as a task. But after doing 3-4 problems with all their brains activities... working out the rest of the problems become a mania. They get addicted to the problem solving

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*and every time they solve a
problem by themselves, their
confident level also increases.”*

*“I am teaching the fundamentals
of Molecular Spectroscopy and
your books represent excellent
sources of spectroscopic*

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problems for students.”

Molecular biology operates at three levels – genes, proteins and metabolites. This book is unique in that it provides a comprehensive description of an approach (metabonomics) to

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characterise the endogenous metabolites in a living system, complementing gene and protein studies (genomics and proteomics). These "omics" methods form the basis for understanding biology at a

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systems level. The Handbook of Metabonomics and Metabolomics aims to be the definitive work on the rapidly expanding subjects of metabolic profiling, metabolite and biomarker identification,

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*encompassing the fields of
metabonomics and
metabolomics. It covers the
principles of the subject, the
analytical and statistical
techniques used and the wide
variety of applications. **

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*comprehensive description of an approach (metabonomics) to characterise the endogenous metabolites in a living system, complementing gene and protein studies * aims to be the definitive work on the rapidly expanding*

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*subjects of metabolic profiling, metabolite and biomarker identification * covers the principles of the subject, the analytical and statistical techniques used and the wide variety of applications.*

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200 and More NMR

Experiments A Practical

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Protein NMR Spectroscopy,

Second Edition combines a

comprehensive theoretical

treatment of NMR spectroscopy

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with an extensive exposition of the experimental techniques applicable to proteins and other biological macromolecules in solution. Beginning with simple theoretical models and experimental techniques, the

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book develops the complete repertoire of theoretical principles and experimental techniques necessary for understanding and implementing the most sophisticated NMR experiments. Important new

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techniques and applications of NMR spectroscopy have emerged since the first edition of this extremely successful book was published in 1996. This updated version includes new sections describing

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*measurement and use of
residual dipolar coupling
constants for structure
determination, TROSY and
deuterium labeling for application
to large macromolecules, and
experimental techniques for*

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characterizing conformational dynamics. In addition, the treatments of instrumentation and signal acquisition, field gradients, multidimensional spectroscopy, and structure calculation are updated and

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enhanced. The book is written as a graduate-level textbook and will be of interest to biochemists, chemists, biophysicists, and structural biologists who utilize NMR spectroscopy or wish to understand the latest

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developments in this field.

*Provides an understanding of the
theoretical principles important
for biological NMR spectroscopy
Demonstrates how to implement,
optimize and troubleshoot
modern multi-dimensional NMR*

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*experiments Allows for the
capability of designing effective
experimental protocols for
investigations of protein
structures and dynamics
Includes a comprehensive set of
example NMR spectra of*

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*ubiquitin provides a reference for
validation of experimental
methods*

*From the initial observation of
proton magnetic resonance in
water and in paraffin, the
discipline of nuclear magnetic*

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resonance has seen unparalleled growth as an analytical method. Modern NMR spectroscopy is a highly developed, yet still evolving, subject which finds application in chemistry, biology, medicine, materials science and

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geology. In this book, emphasis is on the more recently developed methods of solution-state NMR applicable to chemical research, which are chosen for their wide applicability and robustness. These have, in

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many cases, already become established techniques in NMR laboratories, in both academic and industrial establishments. A considerable amount of information and guidance is given on the implementation and

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*execution of the techniques
described in this book.*

*"The book contains twenty three
chapters written by experts on
the subject is structured in two
parts: the first one describes the
role of the latest developments in*

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analytical and bioanalytical techniques, and the second one deals with the most innovative applications and issues in food analysis. The two first introductory chapters about sampling technique, from basic

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*one to the most recent
advances, which is still a food
challenge because is responsible
of the quality and assurance of
the analysis, and on data analysis
and chemometrics are followed
by a review of the most recently*

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*applied techniques in process
(on-line) control and in
laboratories for the analysis of
major or minor compounds of
food. These techniques ranged
from the non-invasive and non-
destructive ones, such as*

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infrared spectroscopy, magnetic resonance and ultrasounds, to emerging areas as nanotechnology, biosensors and electronic noses and tongues, including those already well-established in food analysis,

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*such as chromatographic
and electrophoretic techniques.
These chapters also include two
important tools for solving
problems in chemical and
biological analysis such as mass
spectrometry and molecular-*

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based techniques"--

[*Protein NMR Spectroscopy*](#)

[*Nuclear Magnetic Resonance*](#)

[*Spectroscopy*](#)

[*Nuclear Magnetic Resonance*](#)

[*Second, Enlarged Edition*](#)

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[Chemical Engineering in the
Pharmaceutical Industry, Active
Pharmaceutical Ingredients
Classics in Spectroscopy
Organic Structures from 2D NMR
Spectra
Introduction to Spectroscopy](#)

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[NMR Spectroscopy Explained](#)
[Annual Reports on NMR](#)
[Spectroscopy](#)

NMR spectroscopy is one of the most important analytical methods available today. This practice-oriented textbook shows how NMR spectra is used in the

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education of organic structures. The emphasis is on practical rather than on theoretical aspects, which are treated only briefly. NMR- From Spectra to Structures is a textbook providing an ideal practical guide to today's standard NMR experiments for students and laboratory personnel.

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The set of 35 graded problems includes not only the 1D NMR spectra (proton, carbon, DEPT/APT) but, for the first time in a textbook, also the most important 2D spectra (H,H and C,H correlation).

Metabolomics, the global characterisation of the small molecule

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complement involved in metabolism, has evolved into a powerful suite of approaches for understanding the global physiological and pathological processes occurring in biological organisms. The diversity of metabolites, the wide range of metabolic pathways and their

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divergent biological contexts require a range of methodological strategies and techniques. Methodologies for Metabolomics provides a comprehensive description of the newest methodological approaches in metabolomic research. The most important technologies used to identify

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and quantify metabolites, including nuclear magnetic resonance and mass spectrometry, are highlighted. The integration of these techniques with classical biological methods is also addressed. Furthermore, the book presents statistical and chemometric methods for evaluation of the resultant

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data. The broad spectrum of topics includes a vast variety of organisms, samples and diseases, ranging from in vivo metabolomics in humans and animals to in vitro analysis of tissue samples, cultured cells and biofluids. Since the development of the NMR spectrometer in the 1950s, NMR

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spectra have been widely used for the elucidation of the 2D structure of newly synthesized and natural compounds. In the 1980s, the high-resolution NMR spectrometer (> 300 Mhz) and 2D experiments were introduced, which opens up the possibility to determine the 3D structure of large molecules,

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especially biomolecules. However, NMR spectroscopy has been rarely applied to drug analysis. This book illustrates the power and versatility of NMR spectroscopy in the determination of impurities in and the content of drugs, the composition of polymer excipients, the

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characterization of isomeric drug mixtures, the complexity of drugs with small-size components or ions, and the behavior of drugs in acid and basic solution. In addition, NMR spectroscopy and especially the hyphenated technique with HPLC is shown to be a powerful tool to

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measure a drug and its metabolites in various body fluids. The solid state NMR technique can give information on the structure, especially the conformation of drugs and excipients in drug formulations. Recently, SAR by NMR, introduced by Fesik, impressively demonstrated the

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potential of NMR spectroscopy in drug development and in the characterization of the interaction between large molecules and ligands. The complexation between proteins, lipids and cyclodextrins with drugs is described. Finally, NMR imaging (MRI and MRS) can be used to characterize

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the liberation of drugs from a drug formulation. Furthermore, the distribution of substances in plants, in animals, in tissues and in humans can be visualized by imaging. In short, this book covers all aspects of drug analysis.

Bioactive natural products are proving

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to be a rich source of novel
therapeutics to both protect against
and combat diseases, as well as serve
as lead compounds in crop protection.
Following the successful format of the
first edition, this volume brings
together collective research from many
new contributors and emphasizes the

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rationale behind the Nuclear Magnetic Resonance (NMR) spectroscopy is a nondestructive technique that can be used to characterize a wide variety of systems. Sustained development of both methodology and instrumentation have allowed NMR to evolve as a powerful

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technology, with applications in pure sciences, medicine, drug development, and important branches of industry. NMR provides precise structural information down to each atom and bond in a molecule, and is the only method for the determination of structures of molecules in a

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solution. This book compiles a series of articles describing the application of NMR in a variety of interesting scientific challenges. The articles illustrate the versatility and flexibility of NMR.

Nuclear magnetic resonance (NMR) is an analytical tool used by chemists

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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

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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. Nuclear magnetic resonance (NMR) is an analytical tool

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Nuclear Magnetic Resonance (NMR) spectroscopy, a physical phenomenon based upon the magnetic properties of certain atomic nuclei, has found a wide range of applications in life sciences over recent decades. The dramatic advances in NMR techniques have led to corresponding advances in the

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ability of NMR to study structure, dynamics and interactions of biological macromolecules in solution under close to physiological conditions. This volume focuses on the use of NMR to study proteins. NMR can be used to determine detailed three-dimensional structures of proteins in solution.

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Furthermore, it provides information about conformational or chemical exchange, internal mobility and dynamics at timescales varying from picoseconds to seconds. It is the primary technique used to obtain information on intrinsically disordered (unfolded) proteins, since these

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proteins will not crystallize easily. NMR is also a very powerful method for the study of interactions of protein with other molecules, whether small molecules (including drugs), nuclear acids or other proteins. This up-to-date volume covers NMR techniques and their application to proteins, with a

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focus on practical details. This book will provide a newcomer to NMR with the practical guidance in order to carry out successful experiments with proteins and to analyze the resulting spectra. Those who are familiar with the chemical applications of NMR will also find is useful in understanding the

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special requirements of protein NMR.

A guide to the development and manufacturing of pharmaceutical products written for professionals in the industry, revised second edition

The revised and updated second edition of Chemical Engineering in the Pharmaceutical Industry is a practical

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book that highlights chemistry and chemical engineering. The book 's regulatory quality strategies target the development and manufacturing of pharmaceutically active ingredients of pharmaceutical products. The expanded second edition contains revised content with many new case

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studies and additional example calculations that are of interest to chemical engineers. The 2nd Edition is divided into two separate books: 1) Active Pharmaceutical Ingredients (API ' s) and 2) Drug Product Design, Development and Modeling. The active pharmaceutical ingredients

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book puts the focus on the chemistry, chemical engineering, and unit operations specific to development and manufacturing of the active ingredients of the pharmaceutical product. The drug substance operations section includes information on chemical reactions,

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mixing, distillations, extractions, crystallizations, filtration, drying, and wet and dry milling. In addition, the book includes many applications of process modeling and modern software tools that are geared toward batch-scale and continuous drug substance pharmaceutical operations.

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This updated second edition: •
Contains 30 new chapters or revised chapters specific to API, covering topics including: manufacturing quality by design, computational approaches, continuous manufacturing, crystallization and final form, process safety • Expanded topics of scale-up,

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continuous processing, applications of thermodynamics and thermodynamic modeling, filtration and drying • Presents updated and expanded example calculations • Includes contributions from noted experts in the field Written for pharmaceutical engineers, chemical engineers,

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undergraduate and graduate students, and professionals in the field of pharmaceutical sciences and manufacturing, the second edition of Chemical Engineering in the Pharmaceutical Industry focuses on the development and chemical engineering as well as operations

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specific to the design, formulation, and manufacture of drug substance and products.

[NMR for Physical and Biological Scientists](#)

[Methodologies for Metabolomics
A Practical Course](#)

[Developments and Applications](#)

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[100 and More Basic NMR](#)

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[Understanding NMR Spectroscopy](#)

[NMR of Quadrupolar Nuclei in Solid](#)

[Materials](#)

[NMR Spectroscopy in Drug](#)

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[Development and Analysis](#)

[Spectroscopic Methods in Organic
Chemistry](#)

[Bioactive Natural Products](#)

This book gives a wide overview of the state-of-the-art applications of Raman spectroscopy in characterization of materials and biomaterials. The Raman

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signal is intrinsically smaller than other vibrational techniques; however, mainly through intensification processes, such as resonance Raman (RR) and surface-enhanced Raman spectroscopy (SERS), the Raman cross section can be strongly amplified. Thoroughly in these signal amplifications, the study of a diversity of

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chemical systems and the use of Raman technique for in situ and in vivo measurements is possible. The main goal of this book is to open up to an extended audience the possibilities of uses of Raman spectroscopy. In fact, this collective work will be beneficial to students, teachers, and researchers of many areas who are

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interested to expand their knowledge about Raman spectroscopy applied to nanotechnology, biotechnology, environmental science, inorganic chemistry, and health sciences.

The first book of its kind to describe the art of NMR using everyday examples. This textbook will not only fascinate students

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wanting to learn about the topic, but also those experienced analytical chemists who are still inspired by their profession. The contents provide for easy reading by using natural products that everyone knows, such as caffeine, backed by an attractive layout with many pictures to visualize the topics. In addition, an in-depth analytical

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part makes the book a valuable teaching tool, or for self-learning using the questions and answers at the end of each chapter.

Nuclear Magnetic Resonance spectroscopy is a dynamic way for scientists of all kinds to investigate the physical, chemical, and biological

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properties of matter. Its many applications make it a versatile tool previously subject to monolithic treatment in reference-style texts. Based on a course taught for over ten years at Brandeis University, this is the first textbook on NMR spectroscopy for a one-semester course or self-instruction. In keeping with the authors' efforts to

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make it a useful textbook, they have included problems at the end of each chapter. The book not only covers the latest developments in the field, such as GOESY (Gradient Enhanced Overhauser Spectroscopy) and multidimensional NMR, but includes practical examples using real spectra and associated problem sets.

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Assuming the reader has a background of chemistry, physics and calculus, this textbook will be ideal for graduate students in chemistry and biochemistry, as well as biology, physics, and biophysics. NMR for Physical and Biological Scientists will also be useful to medical schools, research facilities, and the many

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chemical, pharmaceutical, and biotech firms that offer in-house instruction on NMR spectroscopy.

The renowned Oxford Chemistry Primers series, which provides focused introductions to a range of important topics in chemistry, has been refreshed and updated to suit the needs of today's

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students, lecturers, and postgraduate researchers. The rigorous, yet accessible, treatment of each subject area is ideal for those wanting a primer in a given topic to prepare them for more advanced study or research. Moreover, cutting-edge examples and applications throughout the texts show the relevance of the chemistry

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being described to current research and industry. The learning features provided, including questions at the end of every chapter and online multiple-choice questions, encourage active learning and promote understanding. Furthermore, frequent diagrams, margin notes, and glossary definitions all help to enhance a

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student's understanding of these essential areas of chemistry. Nuclear Magnetic Resonance offers a concise and accessible introduction to the physical principles of liquid-state NMR, a powerful technique for probing molecular structures.

Examples, applications, and exercises are provided throughout to enable beginning

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undergraduates to get to grips with this important analytical technique. Online Resource Centre The Online Resource Centre to accompany Nuclear Magnetic Resonance features: For registered adopters of the text: * Figures from the book available to download For students: * Multiple-choice questions for self-

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directed learning * Full worked solutions
to the end-of-chapter exercises

This book is a well-established guide to
the interpretation of the mass, ultraviolet,
infrared and nuclear magnetic resonance
spectra of organic compounds. It is
designed for students of organic chemistry
taking a course in the application of these

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techniques to structure determination. The text also remains useful as a source of data for organic chemists to keep on their desks throughout their career. In the seventh edition, substantial portions of the text have been revised reflecting knowledge gained during the author's teaching experience over the last seven

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years. The chapter on NMR has been divided into two separate chapters covering the 1D and 2D experiments. The discussion is also expanded to include accounts of the physics at a relatively simple level, following the development of the magnetization vectors as each pulse sequence is introduced. The emphasis on

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the uses of NMR spectroscopy in structure determination is retained. Worked examples and problem sets are included on a chapter level to allow students to practise their skills by determining the chemical structures of unknown compounds.

This text is aimed at people who have

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some familiarity with high-resolution NMR and who wish to deepen their understanding of how NMR experiments actually 'work'. This revised and updated edition takes the same approach as the highly-acclaimed first edition. The text concentrates on the description of commonly-used experiments and explains

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in detail the theory behind how such experiments work. The quantum mechanical tools needed to analyse pulse sequences are introduced set by step, but the approach is relatively informal with the emphasis on obtaining a good understanding of how the experiments actually work. The use of two-colour

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printing and a new larger format improves the readability of the text. In addition, a number of new topics have been introduced: How product operators can be extended to describe experiments in AX2 and AX3 spin systems, thus making it possible to discuss the important APT, INEPT and DEPT experiments often used

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in carbon-13 NMR. Spin system analysis i.e. how shifts and couplings can be extracted from strongly-coupled (second-order) spectra. How the presence of chemically equivalent spins leads to spectral features which are somewhat unusual and possibly misleading, even at high magnetic fields. A discussion of

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chemical exchange effects has been introduced in order to help with the explanation of transverse relaxation. The double-quantum spectroscopy of a three-spin system is now considered in more detail. Reviews of the First Edition "For anyone wishing to know what really goes on in their NMR experiments, I would

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highly recommend this book" – Chemistry World "...I warmly recommend for budding NMR spectroscopists, or others who wish to deepen their understanding of elementary NMR theory or theoretical tools" – Magnetic Resonance in Chemistry With a foreword by J. D. Roberts Written by an NMR expert with long-standing

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teaching experience, the first edition of this textbook has been a huge success. New features of this thoroughly revised and substantially enlarged second edition include * NMR spectroscopy of nuclides other than ^1H and ^{13}C * 'reverse' procedures for recording spectra
Chemists, biologists, physicians,

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pharmacists and technical assistants will find this new edition even more useful for their daily work. From reviews of the first edition: 'This book is a pleasure to read and if it does not arouse the student's interest, then it is difficult to see what could. It is clearly written and illustrated ... good value and essential reading for

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anyone wanting to know more about NMR.' Chemistry in Britain 'Another paperback that I would advise students to buy ... [it] can be recommended for general purchase by all chemists.' New Scientist

As a spectroscopic method, nuclear magnetic resonance (NMR) has seen

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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

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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: ¹³C-NMR of Proteins and

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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.

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[Modern Methods in Solid-state NMR](#)
[Simplified Theory, Applications and](#)
[Examples for Organic Chemistry and](#)
[Structural Biology](#)
[Practical Techniques and Applications](#)
[Experimental Strategies and Techniques](#)
[The Handbook of Metabonomics and](#)

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[Metabolomics](#)

[A Detailed Guide](#)

[Volume 45](#)

[Essential Practical NMR for Organic
Chemistry](#)

[An Experimental Approach](#)

[Modern NMR Techniques for Chemistry
Research](#)

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Introduce your students to the latest advances in spectroscopy with the text that has set the standard in the field for more than three decades: INTRODUCTION TO SPECTROSCOPY, 5e, by Donald L. Pavia, Gary M.

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Lampman, George A. Kriz, and James R. Vyvyan. Whether you use the book as a primary text in an upper-level spectroscopy course or as a companion book with an organic chemistry text, your students will receive an

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unmatched, systematic
introduction to spectra and
basic theoretical concepts
in spectroscopic methods.
This acclaimed resource
features up-to-date spectra;
a modern presentation of one-
dimensional nuclear magnetic

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resonance (NMR)
spectroscopy; an
introduction to biological
molecules in mass
spectrometry; and coverage
of modern techniques
alongside DEPT, COSY, and
HECTOR. Important Notice:

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The volume focuses on topics relevant to the developing field of "NMR

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crystallography", that is the use of solids NMR as a complement to diffraction crystallography, and will be of interest to every solid-state NMR researcher working in the chemical sciences. The volumes of this classic

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series, now referred to simply as "Zechmeister" after its founder, L. Zechmeister, have appeared under the Springer Imprint ever since the series' inauguration in 1938. It is therefore not really

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surprising to find out that the list of contributing authors, who were awarded a Nobel Prize, is quite long: Kurt Alder, Derek H.R. Barton, George Wells Beadle, Dorothy Crowfoot-Hodgkin, Otto Diels, Hans von Euler-

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Chelpin, Paul Karrer, Luis
Federico Leloir, Linus
Pauling, Vladimir Prelog,
with Walter Norman Haworth
and Adolf F.J. Butenandt
serving as members of the
editorial board. The volumes
contain contributions on

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various topics related to the origin, distribution, chemistry, synthesis, biochemistry, function or use of various classes of naturally occurring substances ranging from small molecules to

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biopolymers. Each contribution is written by a recognized authority in his field and provides a comprehensive and up-to-date review of the topic in question. Addressed to biologists, technologists

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and chemists alike, the series can be used by the expert as a source of information and literature citations and by the non-expert as a means of orientation in a rapidly developing discipline.

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Learn vital information about drug-DNA interactions from *Drug-DNA Interactions: Structures and Spectra*, the only comprehensive book written about this topic. Understand the types of structural and bonding

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information that can be obtained using specific physico-chemical methods and discover how to design new drugs that are more effective than current treatments and have fewer side effects. Find detailed

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information about X-ray
crystallography, NMR
spectroscopy, molecular
modeling, and optical
spectroscopy such as UV-
Visible absorption,
fluorescence, circular
dichroism (CD), flow linear

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dichroism (FLD), infrared (IR) and Raman spectroscopy. NMR Spectroscopy Explained : Simplified Theory, Applications and Examples for Organic Chemistry and Structural Biology provides a fresh, practical guide to

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NMR for both students and practitioners, in a clearly written and non-mathematical format. It gives the reader an intermediate level theoretical basis for understanding laboratory applications, developing

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concepts gradually within
the context of examples and
useful experiments.

Introduces students to
modern NMR as applied to
analysis of organic
compounds. Presents material
in a clear, conversational

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style that is appealing to students. Contains comprehensive coverage of how NMR experiments actually work. Combines basic ideas with practical implementation of the spectrometer. Provides an

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intermediate level
theoretical basis for
understanding laboratory
experiments. Develops
concepts gradually within
the context of examples and
useful experiments.
Introduces the product

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operator formalism after
introducing the simpler (but
limited) vector model.

The book presents
developments and
applications of these
methods, such as NMR, mass,
and others, including their

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applications in
pharmaceutical and
biomedical analyses. The
book is divided into two
sections. The first section
covers spectroscopic
methods, their applications,
and their significance as

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characterization tools; the second section is dedicated to the applications of spectrophotometric methods in pharmaceutical and biomedical analyses. This book would be useful for students, scholars, and

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scientists engaged in
synthesis, analyses, and
applications of
materials/polymers.

How do the pulse sequences
of modern NMR work? Which
experiment conveys the
desired information? How can

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the maximal amount of information be retrieved from measured spectra? Have you ever been confronted with questions like these? Get the answers and explore the full productivity of your NMR equipment! This

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book is a reliable guide through the maze of modern NMR tools. Written by leading experts, it describes more than a hundred NMR experiments including selective pulses, field gradients and the

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second and third dimension.
Being textbook as well as
reference book for the
laboratory, this book is a
must for every scientist
working with NMR as well as
for students preparing for
their lab courses.

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This book describes the use of NMR spectroscopy for dealing with problems of small organic molecule structural elucidation. It features a significant amount of vital chemical shift and coupling

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information but more importantly, it presents sound principles for the selection of the techniques relevant to the solving of particular types of problem, whilst stressing the importance of extracting the

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maximum available

information from the simple
1-D proton experiment and of
using this to plan
subsequent experiments.

Proton NMR is covered in
detail, with a description
of the fundamentals of the

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technique, the instrumentation and the data that it provides before going on to discuss optimal solvent selection and sample preparation. This is followed by a detailed study of each of the important

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classes of protons, breaking the spectrum up into regions (exchangeables, aromatics, heterocyclics, alkenes etc.). This is followed by consideration of the phenomena that we know can leave chemists struggling;

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chiral centres, restricted rotation, anisotropy, accidental equivalence, non-first-order spectra etc.

Having explained the potential pitfalls that await the unwary, the book then goes on to devote

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chapters to the chemical techniques and the most useful instrumental ones that can be employed to combat them. A discussion is then presented on carbon-13 NMR, detailing its pros and cons and showing how it can

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be used in conjunction with proton NMR via the pivotal 2-D techniques (HSQC and HMBC) to yield vital structural information. Some of the more specialist techniques available are then discussed, i.e. flow

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NMR, solvent suppression,
Magic Angle Spinning, etc.
Other important nuclei are
then discussed and useful
data supplied. This is
followed by a discussion of
the neglected use of NMR as
a tool for quantification

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and new techniques for this explained. The book then considers the safety aspects of NMR spectroscopy, reviewing NMR software for spectral prediction and data handling and concludes with a set of worked Q&As.

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Structures and Spectra

Modern NMR Techniques for
Synthetic Chemistry

Principles of Instrumental
Analysis

200 and More NMR Experiments
Spectroscopic Analyses

Progress in the Chemistry of

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