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Solving Problems with NMR Spectroscopy, Second Edition, is a fully updated and revised version of the best-selling book. This new edition still clearly presents the basic principles and applications of NMR spectroscopy with only as much math as is necessary. It shows how to solve chemical structures with NMR by giving many new, clear examples for readers to understand and try, with new solutions provided in the text. It also explains new developments and concepts in NMR spectroscopy, including sensitivity problems (hardware and software solutions) and an extension of the multidimensional coverage to 3D NMR. The book also includes a series of applications showing how NMR is used in real life to solve advanced problems beyond simple small-molecule chemical analysis. This new text enables organic chemistry students to choose the most appropriate NMR techniques to solve specific structures. The problems provided by the authors help readers understand the discussion more clearly and the solution and interpretation of spectra help readers become proficient in the application of important, modern 1D, 2D, and 3D NMR techniques to structural studies. Explains and presents the most important NMR techniques used for structural determinations Offers a unique problem-solving approach for readers to understand how to solve structure problems Uses questions and problems, including discussions of their solutions and interpretations, to help readers understand the fundamentals and applications of NMR Avoids use of extensive mathematical formulas and clearly explains how to implement NMR structure analysis Foreword by Nobel Prize winner Richard R. Ernst New to This Edition Key developments in the field of NMR spectroscopy since the First Edition in 1996 New chapter on sensitivity enhancement, a key driver of development in NMR spectroscopy New concepts such as Pulse Field Gradients, shaped pulses, and DOSY (Diffusion Order Spectroscopy) in relevant chapters More emphasis on practical aspects of NMR spectroscopy, such as the use of Shigemi tubes and various types of cryogenic probes Over 100 new problems and questions addressing the key concepts in NMR spectroscopy Improved figures and diagrams More than 180 example problems to solve, with detailed solutions provided at the end of each chapter

In Vivo NMR Spectroscopy Robin A. de Graaf Department of in vivo NMR, Utrecht University, The Netherlands This is the first book in the field of in vivo NMR to cover in depth the technical and basic biophysical aspects of the technique. The contents of the book are appropriate to both beginners and experienced users of in vivo NMR spectroscopy. The book has also a practical setup, allowing readers to incorporate the presented concepts into their own MR research. An extensive treatment of radiofrequency pulses is given, together with several tables and recipes for their generation. A practical approach is followed in describing spatial localization and the pros and cons of all known water-suppression techniques. In addition, 2-D NMR, magnetic resonance imaging, spectroscopic imaging, spectral editing and many basic principles are explained and illustrated using practical examples. Several tables containing basic biophysical information, such as resonance frequencies, diffusion coefficients, relaxation constants, and absolute concentrations are also presented. The educational and practical character of this book makes it ideal for use in training courses at large research institutes and academic hospitals. In general, all those involved in fundamental and/or diagnostic in vivo NMR will find this book useful. This can range from people working in dedicated in vivo NMR institutes to radiologists working in hospitals. Also, those who want to broaden their knowledge on the concepts of NMR, such as researchers in high-resolution NMR, neurology, physiology, chemistry, and medical biology will benefit greatly from this book.

I. GENERAL When a sample containing hydrogen is placed in the Although it is assumed that the reader has been exposed static magnetic field, each hydrogen nucleus will precess to the elementary theory of NMR and to the operation at a frequency determined by the magnetic field it of an NMR spectrometer, a brief review of some of the actually experiences. This field, in turn, is determined by basic concepts and definitions will indicate the point of the electronic, and therefore the chemical, environment view used in this book and clarify some of the defini of the nucleus. Thus the variety of chemical environ tions. The discussion is confined to the hydrogen-l iso ments that exist in a molecule will produce a spectrum tope because this is by far the most generally used and, of precession frequencies that will indicate the chemical consequently, far more data are available for it than for nature of the various parts of the molecule. The remain any other isotope. This wealth of data, in turn, leads to ing problem is to observe this spectrum of frequencies. the most accurate and comprehensive set of spectra There are two general methods of observing the structure correlations. spectrum.

For several years we have been organizing seminars and workshops on the application of modem one and two-dimensional NMR methods at the faculty of chemistry in the Ruhr-University Bochum, FRG, and elsewhere, addressing researchers and graduate students who work in the field of organic and natural products chemistry. In 1987, we wrote a workbook (StrukturaufkUirung mit modemer NMR-Spektroskopie, Steinkopff, Darmstadt, FRG, 1988) in German language based on our experience in these courses. Many of the exercises described therein have been used in such courses and some of them have been shaped by the participants to a great extent. The response of readers and discussions with colleagues from many countries encouraged us to produce an English translation in order to make the book accessible to a wider audience. Moreover, the content has been increased from 20 exercise examples in the German, to 23 in the English version. This book could not have been written in the present form without the help of a number of col leagues and, therefore, we acknowledge gratefully the generous supply of samples from and useful discussions with B. Abegaz (Addis Ababa, Ethiopia), U.H. Brinker (Bingham, New York, USA), E.

During the last few years, routine applications of NMR (Nuclear Magnetic Resonance) techniques have developed at a tremendous pace. The latest generation of spectrometers have enabled chemists to perform new types of experiments, such as spinlock and inverse-detected methods. This third, revised and expanded edition introduces the latest methodologies and incorporates them into new exercises.

This handbook provides a straightforward introduction to spectroscopy, showing what it can do and how it does it, together with a clear, integrated and objective account of the wealth of information that can be derived from spectra. The sequence of chapters covers a wide range of the electromagnetic spectrum, and the physical processes involved, from nuclear phenomena to molecular rotation processes. - A day-by-day laboratory guide: its design based on practical knowledge of spectroscopists at universities, industries and research institutes - A well-structured information source containing methods and applications sections framed by sections on general topics - Guides users to a decision about which spectroscopic method and which instrumentation will be the most appropriate to solve their own practical problem - Rapid access to essential information - Correct analysis of a huge number of measured spectra data and smart use of such information sources as databases and spectra libraries

Protein NMR Spectroscopy, Second Edition combines a comprehensive theoretical treatment of NMR spectroscopy 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 book develops the complete repertoire of theoretical principles and experimental techniques necessary for understanding and implementing the most sophisticated NMR experiments. Important new 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 measurement and use of residual dipolar coupling constants for structure determination, TROSY and deuterium labeling for application to large macromolecules, and experimental techniques for characterizing conformational dynamics. In addition, the treatments of instrumentation and signal acquisition, field gradients, multidimensional spectroscopy, and structure calculation are updated and 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 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 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 ubiquitin provides a reference for validation of experimental methods

In recent years high-resolution nuclear magnetic resonance spec troscopy has found very wide application in organie chemistry in structural and physicochemical investigations and. also in the study of the characteristics of organic compounds which are re lated to the distribution of the electron cloud in the molecules. The vigorous development of this method, which may really be re garded as an independent branch of science, is the result of ex tensive progress in NMR technology, the refinement of its theory, and the accumulation of large amounts of experimental material, which has been correlated by empiricallaws and principles. The literature directly concerned with the NMR method and its applica tion has now grown to such an extent that a complete review of it is practically impossible. Therefore the authors have limited themselves to an examination of only the most important, funda mental, and general investigations. The book consists of six chapters. In the first chapter we have attempted to present the fundamentals of the NMR method in such a way that the reader with little knowledge of the subject will be able to use the method in practical work for investigating simple compounds and solving simple problems. The three subsequent chapters give a deeper analysis of the method, while the last two chapters and the appendix illustrate the various applications of NMR spectroscopy in organic chemistry.

Combines clear and concise discussions of key NMR concepts with succinct and illustrative examples Designed to cover a full course in Nuclear Magnetic Resonance (NMR) Spectroscopy, this text offers complete coverage of classic (one-dimensional) NMR as well as up-to-date coverage of two-dimensional NMR and other modern methods. It contains practical advice, theory, illustrated applications, and classroom-tested problems; looks at such important ideas as relaxation, NOEs, phase cycling, and processing parameters; and provides brief, yet fully comprehensible, examples. It also uniquely lists all of the general parameters for many experiments including mixing times, number of scans, relaxation times, and more. Nuclear Magnetic Resonance Spectroscopy: An Introduction to Principles, Applications, and Experimental Methods, 2nd Edition begins by introducing readers to NMR spectroscopy - an analytical technique used in modern chemistry, biochemistry, and biology that allows identification and characterization of organic, and some inorganic, compounds. It offers chapters covering: Experimental Methods; The Chemical Shift; The Coupling Constant; Further Topics in One-Dimensional NMR Spectroscopy; Two-Dimensional NMR Spectroscopy; Advanced Experimental Methods; and Structural Elucidation. Features classical analysis of chemical shifts and coupling constants for both protons and other nuclei, as well as modern multi-pulse and multi-dimensional methods Contains experimental procedures and practical advice relative to the execution of NMR experiments Includes a chapter-long, worked-out problem that illustrates the application of nearly all current methods Offers appendices containing the theoretical basis of NMR, including the most modern approach that uses product operators and coherence-level diagrams By offering a balance between volumes aimed at NMR specialists and the structure-determination-only books that focus on synthetic organic chemists, Nuclear Magnetic Resonance Spectroscopy: An Introduction to Principles, Applications, and Experimental Methods, 2nd Edition is an excellent text for students and post-graduate students working in analytical and bio-sciences, as well as scientists who use NMR spectroscopy as a primary tool in their work.

Spectroscopy is used in physical and analytical chemistry for the identification of substances through the spectrum emitted from or absorbed by them. The derivation of structural information from spectroscopic data is now an integral part of many courses in chemistry and related subjects

at most universities. This workbook: Features exercises to help develop the student's understanding of how structures are determined from spectra and to promote the student's own interpretation of different spectra. Covers a large range of spectroscopic data, including mass spectrometry, infrared and 1H and 13C nuclear magnetic resonance, typically used in the routine analysis of small--sized organic molecules. Presents in full-color, in a workbook-friendly format the spectra for interpretation with explanations and analyses on the facing page. Related to the workbook the authors have an online resource of the problems featured in the workbook, available at: htttp://spectros.unice.fr/ By using the print edition alongside the online spectra, students will be able to enhance their understanding of the interpretation of multiple spectra.

Through numerous examples, the principles of the relationship between chemical structure and the NMR spectrum are developed in a logical, step-by-step fashion Includes examples and exercises based on real NMR data including full 600 MHz one- and two-dimensional datasets of sugars, peptides, steroids and natural products Includes detailed solutions and explanations in the text for the numerous examples and problems and also provides large, very detailed and annotated sets of NMR data for use in understanding the material Describes both simple aspects of solution-state NMR of small molecules as well as more complex topics not usually covered in NMR books such as complex splitting patterns, weak long-range couplings, spreadsheet analysis of strong coupling patterns and resonance structure analysis for prediction of chemical shifts Advanced topics include all of the common two-dimensional experiments (COSY, ROESY, NOESY, TOCSY, HSQC, HMBC) covered strictly from the point of view of data interpretation, along with tips for parameter settings

Nuclear magnetic resonance (NMR) spectroscopy is one of the most powerful and widely used techniques in chemical research for investigating structures and dynamics of molecules. Advanced methods can even be utilized for structure determinations of biopolymers, for example proteins or nucleic acids. NMR is also used in medicine for magnetic resonance imaging (MRI). The method is based on spectral lines of different atomic nuclei that are excited when a strong magnetic field and a radiofrequency transmitter are applied. The method is very sensitive to the features of molecular structure because also the neighboring atoms influence the signals from individual nuclei and this is important for determining the 3D-structure of molecules. This new edition of the popular classic has a clear style and a highly practical, mostly non-mathematical approach. Many examples are taken from organic and organometallic chemistry, making this book an invaluable guide to undergraduate and graduate students of organic chemistry, biochemistry, spectroscopy or physical chemistry, and to researchers using this well-established and extremely important technique. Problems and solutions are included.

Solid-state NMR covers an enormous range of material types and experimental techniques. Although the basic instrumentation and techniques of solids NMR are readily accessible, there can be significant barriers, even for existing experts, to exploring the bewildering array of more sophisticated techniques. In this unique volume, a range of experts in different areas of modern solid-state NMR explain about their area of expertise, emphasising the “practical aspects” of implementing different techniques, and illustrating what questions can and cannot be addressed. Later chapters address complex materials, showing how different NMR techniques discussed in earlier chapters can be brought together to characterise important materials types. The volume as a whole focusses on topics relevant to the developing field of “NMR crystallography” – the use of solids NMR as a complement to diffraction crystallography. This book is an ideal complement to existing introductory texts and reviews on solid-state NMR. New researchers wanting to understand new areas of solid-state NMR will find each chapter to be the equivalent to spending time in the laboratory of an internationally leading expert, learning the hints and tips that make the difference between knowing about a technique and being ready to put it into action. With no equivalent on the market, it will be of interest to every solid-state NMR researcher (academic and postgraduate) working in the chemical sciences.

The organic chemist who wishes to learn how to use NMR spectra effectively must first learn the essential facts and then must gain both ability and confidence through the solution of a wide range of specific problems. My previous volume, Interpretation of NMR Spectra: An Empirical Approach, was written specifically to present and explain the necessary background material. The present volume is designed to provide the reader with a full range of experience in the interpretation of NMR spectra. The exercises are arranged in a sequence designed for rapid assimila tion of not only the basic concepts, but also increasingly more complex details. Emphasis is placed on the difficulties normally encountered in the use of spectra and also on the many practical aids which are helpful in overcoming these difficulties. For most of the problems, at least one reasoning process is outlined by which the questions can be answered. This text is, in part, an outgrowth of my participation in workshops which were held at Canisius College under the direction of Dr. Herman Szymanski and at the College of Pharmacy of the University of Illinois under the direction of Dr. Charles L. Bell v and Dr. Ludwig Bauer. This experience has been of considerable aid in the formulation of this workbook. Most of the spectra used in this book were obtained by Searle staff members in the course of their own research.

Introduction to NMR Spectroscopy R. J. Abraham, School of Chemistry, University of Liverpool J. Fisher, Biological NMR Centre, University of Leicester P. Loftus, Stuart Pharmaceuticals, Delaware, USA This book is a new, extended edition of Proton and Carbon 13 NMR by R. J. Abraham and P. Loftus. The initial chapters cover the fundamentals of NMR spectroscopy commencing with an explanation of how the nuclear magnetic response occurs, followed by a detailed discussion of chemical shifts and coupling constants, parameters not discussed to any length in other textbooks aimed at a similar level of interest. Emphasis is given to the vectorial description of multipulse experiments, as this is probably the easiest way to grasp how different information may be gained simply by changing a pulse sequence. An understanding of multipulse NMR is a prerequisite for understanding 2D NMR. The section on 2D NMR begins with a discussion of the resolved experiment. This is a logical initial choice as the spectra produced by this experiment may be readily compared with 1D spectra. Following on from this both heteronuclear and homonuclear correlation spectroscopy are described and examples given. The final section of the book should be considered as an applications section. It is aimed at showing the reader that NMR is not just of use to the synthetic organic chemist but is also of use to biochemists for investigating the solution state structure and function of proteins, enzymes, etc. The application of high resolution NMR to the solid state is also discussed, thereby indicating the developments which have taken place as far as spectrometer hardware is concerned.

This text is aimed at people who have 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 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 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 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 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 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

Following its well-received predecessor, this book offers an essential guide to chemists for understanding fluorine in spectroscopy. With over 1000 compounds and 100 spectra, the second edition adds new data – featuring fluorine effects on nitrogen NMR, chemical shifts, and coupling constants. • Explains how to successfully incorporate fluorine into target molecules and utilize fluorine substituents to structurally characterize organic compounds • Includes new data on nitrogen NMR, focusing on N-15, to portray the influence of fluorine upon nitrogen NMR chemical shifts and coupling constants • Expands on each chapter from the first edition with additional data and updated discussion from recent findings • "The flawless ordering of material covered in this stand-alone volume is such that information can be found very easily." – Angewandte Chemie review of the first edition, 2010

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.

Keeping mathematics to a minimum, this book introduces nuclear properties, nuclear screening, chemical shift, spin-spin coupling, and relaxation. It is one of the few books that provides the student with the physical background to NMR spectroscopy from the point of view of the whole of the periodic table rather than concentrating on the narrow applications of 1H and 13C NMR spectroscopy. Aids to structure determination, such as decoupling, the nuclear Overhauser effect, INEPT, DEPT, and special editing, and two dimensional NMR spectroscopy are discussed in detail with examples, including the complete assignment of the 1H and 13C NMR spectra of D-amygdain. The authors examine the requirements of a modern spectrometer and the effects of pulses and discuss the effects of dynamic processes as a function of temperature or pressure on NMR spectra. The book concludes with chapters on some of the applications of NMR spectroscopy to medical and non-medical imaging techniques and solid state chemistry of both I = F1/2 and I > F1/2 nuclei. Examples and problems, mainly from the recent inorganic/organometallic chemistry literature support the text throughout. Brief answers to all the problems are provided in the text with full answers at the end of the book.

Applications of NMR Spectroscopy is a book series devoted to publishing the latest advances in the applications of nuclear magnetic resonance (NMR) spectroscopy in various fields of organic chemistry, biochemistry, health and agriculture. The seventh volume of the series features six reviews focusing on NMR spectroscopic techniques for studying structures of protein complexes, metabolic profiling of gut bacteria, lipid digestion, lung disorders, and early cancer diagnosis, respectively.

This book describes the advanced developments in methodology and applications of NMR spectroscopy to life science and materials science. Experts who are leaders in the development of new methods and applications of life and material sciences have contributed an exciting range of topics that cover recent advances in structural determination of biological and material molecules, dynamic aspects of biological and material molecules, and development of novel NMR techniques, including resolution and sensitivity enhancement. First, this book particularly emphasizes the experimental details for new researchers to use NMR spectroscopy and pick up the potentials of NMR spectroscopy. Second, the book is designed for those who are involved in either developing the technique or expanding the NMR application fields by applying them to specific samples. Third, the Nuclear Magnetic Resonance Society of Japan has organized this book not only for NMR members of Japan but also for readers worldwide who are interested in using NMR spectroscopy extensively.

This book is for those familiar with solution-state NMR who are encountering solid-state NMR for the first time. It presents the current understanding and applications of solid-state NMR with a rigorous but readable approach, making it easy for someone who merely wishes to gain an overall impression of the subject without details. This dual requirement is met through careful construction of the material within each chapter. The book is divided into two parts: "Fundamentals" and "Further Applications." The section on Fundamentals contains relatively long chapters that deal with the basic theory and practice of solid-state NMR. The essential differences and extra scope of solid-state NMR over solution-state is dealt with in an introductory chapter. The basic techniques that all chapters rely on are collected into a second chapter to avoid unnecessary repetition later. Remaining chapters in the "Fundamentals" part deal with the major areas of solid-state NMR which all solid-state NMR spectroscopists should know about. Each begins with an overview of the topic that puts the chapter in context. The basic principles upon which the techniques in the chapter rely are explained in a separate section. Each of these chapters exemplifies the principles and techniques with the applications most commonly found in current practice. The "Further Applications" section contains a series of shorter chapters which describe the NMR techniques used in other, more specific areas. The basic principles upon which these techniques rely will be expounded only if not already in the Fundamentals part.

Presents basic concepts, experimental methodology and data acquisition, and processing standards of in vivo NMR spectroscopy This book covers, in detail, the technical and biophysical aspects of in vivo NMR techniques and includes novel developments in the field such as hyperpolarized NMR, dynamic 13C NMR, automated shimming, and parallel acquisitions. Most of the techniques are described from an educational point of view, yet it still retains the practical aspects appreciated by experimental NMR spectroscopists. In addition, each chapter concludes with a num-

ber of exercises designed to review, and often extend, the presented NMR principles and techniques. The third edition of In Vivo NMR Spectroscopy: Principles and Techniques has been updated to include experimental detail on the developing area of hyperpolarization; a description of the semi-LASER sequence, which is now a method of choice; updated chemical shift data, including the addition of 31P data; a troubleshooting section on common problems related to shimming, water suppression, and quantification; recent developments in data acquisition and processing standards; and MatLab scripts on the accompanying website for helping readers calculate radiofrequency pulses. Provide an educational explanation and overview of in vivo NMR, while maintaining the practical aspects appreciated by experimental NMR spectroscopists Features more experimental methodology than the previous edition End-of-chapter exercises that help drive home the principles and techniques and offer a more in-depth exploration of quantitative MR equations Designed to be used in conjunction with a teaching course on the subject In Vivo NMR Spectroscopy: Principles and Techniques, 3rd Edition is aimed at all those involved in fundamental and/or diagnostic in vivo NMR, ranging from people working in dedicated in vivo NMR institutes, to radiologists in hospitals, researchers in high-resolution NMR and MRI, and in areas such as neurology, physiology, chemistry, and medical biology.

From the initial observation of proton magnetic resonance in water and in paraffin, the discipline of nuclear magnetic 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 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 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 execution of the techniques described in this book.

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 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 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 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 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; 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 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 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 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 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.

Clear, accessible coverage of modern NMR spectroscopy-for students and professionals in many fields of science Nuclear magnetic resonance (NMR) spectroscopy has made quantum leaps in the last decade, becoming a staple tool in such divergent fields as chemistry, physics, materials science, biology, and medicine. That is why it is essential that scientists working in these areas be fully conversant with current NMR theory and practice. This down-to-basics text offers a comprehensive, up-to-date treatment of the fundamentals of NMR spectroscopy. Using a straightforward approach that develops all concepts from a rudimentary level without using heavy mathematics, it gives readers the knowledge they need to solve any molecular structure problem from a complete set of NMR data. Topics are illustrated throughout with hundreds of figures and actual spectra. Chapter-end summaries and review problems with answers are included to help reinforce and test understanding of key material. From NMR studies of biologically important molecules to magnetic resonance imaging, this book serves as an excellent all-around primer on NMR spectroscopic analysis.

R.N.IBBETT This book provides a source of information on all major aspects of NMR spectroscopy of synthetic polymers. It represents a deliberate attempt to pull together the numerous strands of the subject in a single comprehensive volume, designed to be readable at every scientific level. It is intended that the book will be of use to the vast majority of polymer scientists and NMR spec troscopists alike. Readers new to NMR will find extensive information within the book on the available techniques, allowing full exploration of the many polymer science applications. Readers already established within a branch of NMR will find the book an excellent guide to the practical study of polymers and the inter pretation of experimental data. Readers who have specialised in polymer NMR will find the book a valuable dictionary of proven methodologies, as well as a guide to the very latest developments in the subject. Workers from all of the main branches of polymer NMR have been invited to contribute. Each chapter therefore contains information relating to a parti cular investigative topic, indentified mainly on the basis of technique. The book is loosely divided between solution and solid-state domains, although the numerous interconnections confirm that these two domains are parts of the same continuum. Basic principles are explained within each chapter, combined with discussions of experimental theory and applications. Examples of polymer investigations are covered generously and in many chapters there are discussions of the most recent theoretical and experimental developments.

NMR is an analytical tool used by chemists and physicists to study the structure and dynamics of molecules. In recent years, no other technique has 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 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 used by chemists 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 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

This is the second edition of a unique book in the field of in vivo NMR covering in detail the technical and biophysical aspects of the technique. The contents of the book are appropriate to both beginners and experienced users of in vivo NMR spectroscopy. The new edition is focussed on bringing the reader practical insights and advice, but is also geared towards use as a study aid and in NMR courses. Recent advances in NMR spectroscopy, like high field NMR, hyperpolarized NMR and new localization and editing techniques have been included. An extensive and updated treatment of radiofrequency pulses is given, together with several tables and recipes for their generation. Solutions to the exercises within this text can be found here

Nuclear magnetic resonsance (NMR) spectrocopy is the most powerful research tool used in chemistry today, but many chemists have yet to realize its true potential. Recent advances in NMR have led to a formidable array of new techniques - and acronyms - which leaves even the professional spectroscopist bewildered. How, then, can chemists decide which approach will solve their particular structural or mechanistic problem? This book provides a non-mathematical, descriptive approach to modern NMR spectroscopy, taking examples from organic, inorganic, and biological chemistry. It also contains much practical advice about the acquisition and use of spectra. Starting from the simple 'one pulse' sequence, the text employs a 'building block' approach to lead naturally to multiple pulse and two-dimensional NMR. Spectra of readily available compounds illustrate each technique. One- and two- dimensional methods are integrated in three chapters which show how to solve problems by making connections between spins through bonds, through space, or through exchange. There are also chapters on spectrum editing and solids. The final chapter contains a case history which attempts to weave the many strands of the text into a coherent strategy. This second edition reflects the progress made by NMR in the past few years; there is a greater emphasis on inorganic nuclei; some two-colour spectra are used; the treatment of heteronuclear experiments has moved from direct to 'inverse' detection; many new examples and spectra have been included; and the literature to early 1992 has been covered. An accompanying text, Modern NMR spectroscopy: A workbook of chemical problems, by Jeremy Sanders, Edwin Constable, and Brian Hunter, is available from OUP. Using a combination of worked examples and set problems, this workbook provides a practical guide to the accurate interpretation of NMR spectra, which will be of value to students and professional scientists alike.

Erros I have made; Interpretation of spectra; Symmetry and exchange; Structure determination using NMR alone; Structure and mechanism; Hints; Solutions.

At a point where most introductory organic chemistry texts end, this problems-based workbook picks up the thread to lead students through a graduated set of 120 problems. With extensive detailed spectral data, it contains a variety of problems designed by renowned authors to develop proficiency in organic structure determination. This workbook leads you from basic problems encountered in introductory organic chemistry textbooks to highly complex natural product-based problems. It presents a concept-based learning platform, introducing key concepts sequentially and reinforcing them with problems that exemplify the complexities and underlying principles that govern each concept. The book is organized in such a way that allows you to work through the problems in order or in selections according to your experience and desired area of mastery. It also provides access to raw data files online that can be downloaded and used for data manipulation using freeware or commercial software. With its problem-centered approach, integrated use of online and digital resources, and appendices that include notes and hints, Problems in Organic Structure Determination: A Practical Approach to NMR Spectroscopy is an outstanding resource for training students and professionals in structure determination.

NMR spectroscopy has proven to be a powerful technique to study the structure and dynamics of biological macromolecules. Fundamentals of Protein NMR Spectroscopy is a comprehensive textbook that guides the reader from a basic understanding of the phenomenological properties of magnetic resonance to the application and interpretation of modern multi-dimensional NMR experiments on 15N/13C-labeled proteins. Beginning with elementary quantum mechanics, a set of practical rules is presented and used to describe many commonly employed multi-dimensional, multi--nuclear NMR pulse sequences. A modular analysis of NMR pulse sequence building blocks also provides a basis for understanding and developing novel pulse programs. This text not only covers topics from chemical shift assignment to protein structure refinement, as well as the analysis of protein dynamics and chemical kinetics, but also provides a practical guide to many aspects of modern spectrometer hardware, sample preparation, experimental set-up, and data processing. End of chapter exercises are included to emphasize important concepts. Fundamentals of Protein NMR Spectroscopy not only offer students a systematic, in-depth, understanding of modern NMR spectroscopy and its application to biomolecular systems, but will also be a useful reference for the experienced investigator.

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful and theoretically complex analytical tool. Basic 1H- and 13C-NMR Spectroscopy provides an introduction to the principles and applications of NMR spectroscopy. Whilst looking at the problems students encounter when using NMR spectroscopy, the author avoids the complicated mathematics that are applied within the field. Providing a rational description of the NMR phenomenon, this book is easy to read and is suitable for the undergraduate and graduate student in chemistry. Describes the fundamental principles of the pulse NMR experiment and 2D NMR spectra Easy to read and written with the undergraduate and graduate chemistry student in mind Provides a rational description of NMR spectroscopy without complicated mathematics

"The second edition of this book comes with a number of new figures, passages, and problems. Increasing the number of figures from 290 to 448 has necessarily added considerable length, weight, and, expense. It is my hope that the book has not lost any of its readability and accessibility. I firmly believe that most of the concepts needed to learn organic structure determination using nuclear magnetic resonance spectroscopy do not require an extensive mathematical background. It is my hope that the manner in which the material contained in this book is presented both reflects and validates this belief"--

NMR Spectroscopy Explained : Simplified Theory, Applications and Examples for Organic Chemistry and Structural Biology provides a fresh, practical guide to 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 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 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 intermediate level theoretical basis for understanding laboratory experiments. Develops concepts gradually within the context of examples and useful experiments. Introduces the product operator formalism after introducing the

simpler (but limited) vector model.

Provides a theoretical introduction to graduate scientists and industrial researchers towards the understanding of the assignment of 1H NMR spectra Discusses, and includes on enclosed CD, one of the best, the fastest and most applicable pieces of NMR prediction software available Allows students of organic chemistry to solve problems on 1H NMR with access to over 500 assigned spectra