Organic Structures From Spectra Solutions

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 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 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 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.

Recent advances in the study of structural and dynamic properties of solutions have provided a molecular picture of solute-solvent interactions. Although the study of thermodynamic as well as electronic properties of solutions have played a role in the development of research on the rate and mechanism of chemical reactions, such macroscopic and microscopic properties are insufficient for a deeper understanding of fast chemical and biological reactions. In order to fill the gap between the two extremes, it is necessary to know how molecules are arranged in solution and how they change their positions in both the short and long range. This book has been designed to meet these criteria. It is possible to develop a sound microscopic picture for reaction dynamics in solution without molecular-level knowledge of how reacting ionic or neutral species are solvated and how rapidly the molecular environment is changing with time. A variety of actual examples is given as to how and when modern molecular approaches can be used to solve specific solution problems. The following tools are discussed: x-ray and neutron diffraction, EXAFS, and XANES, molecular dynamics and Monte Carlo computer simulations, Raman, infrared, NMR, fluorescence, and photoelectron emission spectroscopic methods, conductance and viscosity measurements, high pressure techniques, and statistical mechanics methods. Static and dynamic properties of ionic solvation, molecular solvation, ion-pair formation, ligand exchange reactions, and typical organic solvents are useful for bridging the gap between classical thermodynamic studies and modern single-molecule studies in the gas phase. The book will be of interest to solution, physical, inorganic, analytical and structural chemists as well as to chemical kineticists.

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Though the format evolved in the first edition remains intact, relevant new additions have been inserted at appropriate places in various chapters of the book. Also included are a number of sample and study problems at the end of each chapter to illustrate the approach to problem solving that involve translations of sets of spectra into chemical structures. Written primarily to stimulate the interest of students in spectroscopy and make them aware of the latest developments in this field, this book begins with a general introduction to electromagnetic radiation and molecular spectroscopy. In addition to the usual topics on IR, UV, NMR and Mass spectrometry, it includes substantial material on the currently useful techniques such as FT-IR, FT-NMR 13C-NMR, 2D-NMR, GC/MS, FAB/MS, Tendem and Negative Ion Mass Spectrometry for students engaged in advanced studies. Finally it gives a detailed account on Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD).

Determination of Organic Structures by Physical Methods, Volume 1 focuses on the processes, methodologies, principles, and approaches involved in the determination of organic structures by physical methods, including infrared light absorption, thermodynamic properties, Raman spectra, and kinetics. The selection first elaborates on the phase properties of small molecules, equilibrium and dynamic properties of large molecules, and optical rotation. Discussions focus on simple acyclic compounds, carbohydrates, steroids, diffusion, viscosity, osmotic pressure, sedimentation velocity, melting and boiling points, and molar volume. The book then examines ultraviolet and visible light absorption, infrared light absorption, Raman spectra, and the theory of magnetic susceptibility. Concerns cover applications to the study of organic compounds, applications to the determination of structure, determination of thermodynamic properties, and experimental methods and evaluation of data. The text ponders on wave-mechanical theory, reaction kinetics, and dissociation constants, including dissociation of molecular addition compounds, principles of reaction kinetics, and valence-bond treatment of aromatic systems. The selection is a valuable source of data for researchers interested in the determination of organic structures by physical methods.

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 student?s understanding of how structures are derived. This book combines the subject matter of a minimal course needed to understand the major spectroscopic techniques with a carefully selected set of 181 structural problems involving the use of all the major techniques and 19 problems specifically dealing with the interpretation of spin-spin coupling in proton NMR spectra. The problems are graded to develop and consolidate the student?s understanding of organic spectroscopy. The accompanying text indicates the level of theory required to tackle the problems. The examples themselves have been carefully selected to include all important structural features and to emphasise connectivity arguments. Many of the compounds were synthesised specifically for this purpose. There are many easier problems than in other collections. Strenuous efforts have been made to ensure that solutions to the 181 structural problems are unambiguous. The second edition of this popular and successful work has been significantly revised and updated, and contains some 70 additional carefully chosen problems. Most problems feature NMR spectra obtained at higher fields than in the first edition and DEPT experiments as well as coupled 13C NMR spectra are included. Five problems are presented in the style of experimental sections of research papers and the Appendix contains two fully worked solutions. Contents Preface Introduction Ultraviolet Spectroscopy Infrared Spectroscopy Mass Spectrometry Nuclear Magnetic Resonance Spectroscopy Miscellaneous Topics Problems Appendix Index

Complete solutions to in-text problems The Student Solutions Manual to accompany The Systematic Identification of Organic Compounds, 8th Edition is an essential resource for any student using the parent text in class. Providing complete solutions to all practice problems provided in the textbook, this book allows you to assess your understanding of difficult material and clarify complex topics. Fully aligned with the text, this book details structures, formulas, mechanisms, and more to help you pinpoint areas of difficulty and focus your study time for more efficient learning.

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 students' understanding of how organic structures are determined from spectra. The book builds on the very successful teaching philosophy of learning by hands-on problem solving; carefully graded examples build confidence and develop and consolidate a student's understanding of organic spectroscopy. Organic Structures from Spectra, 6th Edition is a carefully chosen set of about 250 structural problems employing the major modern spectroscopic techniques, including Mass Spectrometry, 1D and 2D 13C and 1H NMR Spectroscopy and Infrared Spectroscopy. There are 25 problems specifically dealing with the interpretation of spin–spin coupling in proton NMR spectra and 10 problems based on the quantitative analysis of mixtures using proton and carbon NMR spectroscopy. The accompanying text is descriptive and only explains the underlying theory at a level that is sufficient to tackle the problems. The text includes condensed tables of characteristic spectral properties covering the frequently encountered functional groups. The examples themselves have been selected to include all important structural features and to emphasise connectivity

arguments and stereochemistry. Many of the compounds were synthesised specifically for this book. In this collection, there are many additional easy problems designed to build confidence and to demonstrate basic principles. The Sixth Edition of this popular textbook: now incorporates many new problems using 2D NMR spectra (C–H Correlation spectroscopy, HMBC, COSY, NOESY and TOCSY); has been expanded and updated to reflect the new developments in NMR spectroscopy; has an additional 40 carefully selected basic problems; 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 spectra including routine 2D C–H correlation, HMBC spectra and DEPT spectra; contains a selection of problems in the style of the experimental section of a research paper; includes examples of fully worked solutions in the appendix; has a complete set of solutions available to instructors and teachers from the authors. Organic Structures from Spectra, Sixth Edition will prove invaluable for students of Chemistry, Pharmacy and Biochemistry taking a first course in Organic Chemistry.

The derivation of structural information from spectroscopic data is now an integral part of 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 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) 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 problems are graded to develop and consolidate a students understanding of 2D NMR spectroscopy. There are many easy problems at the beginning of the collection, to build confidence and demonstrate the 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 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 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 – 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 31P, 15N and 19F Organic Structures from 2D NMR Spectrais 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 Chemistry, Pharmacy, Biochemistry and those taking courses in Organic Chemistry. Organic Structures from 2D NMR Spectra is complimented by the Instructors Guide and Solutions Manual to Organic Structures from 2D NMR Spectra which is a set of step–by–step worked solutions to every problem in the book. While it is absolutely clear that there are many ways to get to the correct solution of any of the problems, the instructors guide contains at least one complete pathway to every one of the questions. In addition, the instructors guide carefully rationalises every peak in every spectrum in relation to the correct structure. The Instructors Guide and Solutions Manual to Organic Structures from 2D NMR Spectra: – Is a complete set of worked solutions to the problems contained in Organic Structures from 2D NMR Spectra. – Provides a step–by–step description of the process to derive structures from spectra as well as annotated 2D spectra indicating the origin of every cross peak. – Highlights common artefacts and re–enforces the important characteristics of the most common techniques 2D NMR techniques including COSY, NOESY, HMBC, TOCSY, CH–Correlation and multiplicity–edited C–H Correlation. This guide is an essential aid to those teachers, lecturers and instructors who use Organic Structures from 2D NMR as a text to teach students of Chemistry, Pharmacy, Biochemistry and those taking courses in Organic Chemistry.

"Organic Structures from Spectra, Fourth Edition is a carefully chosen set of more than 280 structural problems employing the major modern spectroscopic techniques, a selection of 18 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 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 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 frequently encountered functional groups."--Jacket.

Solving Problems with NMR Spectroscopy 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 clear examples and solutions. This text will enable organic chemistry students to choose the most appropriate NMR techniques to solve specific structures. The problems to work and the discussion of their solutions and interpretations will help readers becomeproficient in the application of important, modern 1D and 2D NMR techniques to structural studies. Key Features * Presents the most important NMR techniques for structural determinations * Offers a unique problem-solving approach * Uses questions and problems, including discussions of their solutions and interpretations, to help readers grasp NMR * Avoids extensive mathematical formulas * Forewords by Nobel Prize winner Richard R. Ernst and Lloyd M. Jackman

At a point where most introductory organic chemistry texts end, this workbook picks up the thread to lead students from basic problems to a graduated set of 120 highly complex problems. The art of organic structure determination can only be mastered through practice exercises displayed in this book. With minimal theoretical content, the workbook contains a sufficient quantity and variety of problems, developed by authors renowned in their fields, so that students will become truly proficient in organic structure determination.

This introductory textbook covers all the major spectroscopic techniques that cover the derivation of structural information from spectroscopic data. It incorporates over 200 carefully selected problems that are graded to develop and consolidate the students understanding of organic spectroscopy and to develop an understanding of how structures are derived. This, the third edition has been thoroughly revised and updated and reflects the many developments in this area. It includes over 50 new problems and presents challenging examples that have been carefully selected to include all-important structural features and to emphasise connectivity arguments. More emphasis on techniques is included in the problems and the advanced NMR topics section is expanded in the areas of decoupling and applications of the nuclear overhauser effect (nOe). Brief and easy-to-read text providing sufficient detail of theory to be able to solve problems without going to excessive depth. Large, graded selection of problems—from the very easy to challenging. Provides hands-on training for the non-expert

First published over 40 years ago, this was the first text on the identification of organic compounds using spectroscopy. This text is now considered to be a classic. This text presents a unified approach to the structure determination of organic compounds based largely on mass spectrometry, infrared (IR) spectroscopy, and multinuclear and multidimensional nuclear magnetic resonance (NMR) spectroscopy. The key strength of this text is the extensive set of practice and real-data problems (in Chapters 7 and 8). Even professional chemists use these spectra as reference data. Spectrometric Identification of Organic Compounds is written by and for organic chemists, and emphasizes the synergistic effect resulting from the interplay of the spectra. This book is characterized by its problem-solving approach with extensive reference charts and tables. The 8th edition of this text maintains its student-friendly writing style - wording throughout has been updated for consistency and to be more reflective of modern usage and methods. Chapter 3 on proton NMR spectroscopy has been overhauled and updated. Also, new information on polymers and phosphorus functional groups has been added to Chapter 2 on IR spectroscopy.

Organic Spectroscopy presents the derivation of structural information from UV, IR, Raman, 1H NMR, 13C NMR, Mass and ESR spectral data in such a way that stimulates interest of students and researchers alike. The application of spectroscopy for structure determination and analysis has seen phenomenal growth and is now an integral part of Organic Chemistry courses. This book provides: -A logical, comprehensive, lucid and accurate presentation, thus making

it easy to understand even through self-study; -Theoretical aspects of spectral techniques necessary for the interpretation of spectra; -Salient features of instrumentation involved in spectroscopic methods; -Useful spectral data in the form of tables, charts and figures; -Examples of spectra to familiarize the reader; -Many varied problems to help build competence ad confidence; -A separate chapter on 'spectroscopic solutions of structural problems' to emphasize the utility of spectroscopy. Organic Spectroscopy is an invaluable reference for the interpretation of various spectra. It can be used as a basic text for undergraduate and postgraduate students of spectroscopy as well as a practical resource by research chemists. The book will be of interest to chemists and analysts in academia and industry, especially those engaged in the synthesis and analysis of organic compounds including drugs, drug intermediates, agrochemicals, polymers and dyes.

Provides instructions and exercises for identifying organic compounds, covering such topics as solubility, mass spectra, classification tests, and infrared spectra.

Organic Structures from SpectraJohn Wiley & Sons

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

Teaches the use of the complementary information afforded by four types of spectrometry for identification of organic compounds: mass, infrared, nuclear magnetic resonance, and ultra violet spectrometry. Throughout, the emphasis is on the relationship between chemical structure and spectral response of the molecule. Each chapter includes problems to facilitate student comprehension and demonstrate practical aspects of the material. Also provided are extensive reference material in charts and tables at the end of each chapter, solved problems, and 50 sets of Spectra of Compounds to be identified. In addition to extensive updating, the Fifth Edition includes a new chapter on New Dimensions in NMR Spectrometry.

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 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 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 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 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 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 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 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 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 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 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 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 Spectroscopy Infrared Spectroscopy Mass Spectrometry Nuclear Magnetic Resonance Spectroscopy 2DNMR Problems Index Reviews from earlier editions "Your book is becoming one of 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 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 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 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 problems for students."

A unique advanced textbook on spectroscopy. This interactive tutorial presents text, software and data in a state-of-the-art introduction to the interpretation of 13C- and 1H-nuclear magnetic resonance, infrared, mass and UV/VIS spectra. Designed as a hands-on guide, the newcomer or student learns not only by reading but by experimenting, using the

powerful software tools and data provided on the accompanying CD-ROM. The software, based on the outstanding SpecTool product, enables you to learn how to interpret molecular spectra correctly, rapidly and easily. Moreover, you can check your progress by working through the examples embedded in this self-study course that demonstrate how to identify an organic compound and to elucidate its structure. All the material and software presented are the essence of the two authors? longstanding teaching experience.

Spectra-Structure Correlation focuses on absorption spectroscopy of organic compounds, including radiation, absorption, and analysis of compounds. The publication first offers information on wavelength classification of absorption spectra; intensities and shapes of absorption bands; mechanisms for the absorption of radiation; and solvent, phase, and temperature effects. The text also focuses on the spectra of hydrocarbons, as well as olefins, cyclopropanes, benzenes, allenes and cumulenes, cyclobutanes, cyclopentanes, and cyclohexanes. The manuscript reviews compounds with oxygen and nitrogen functions. Discussions focus on aldehydes and ketones, alcohols, carboxylic acids, phenols, ethers and peroxides, acid derivatives, amides and imides, amines, and nitriles and related functions. The text also ponders on organic compounds containing halogen, sulfur, phosphorus, silicon, or boron, inorganic compounds, and complex materials. Concerns include polymers, steroids, purines, pyrimidines, nucleic acids, amino acids, polypeptides, and proteins. The publication is a dependable reference for readers interested in absorption spectroscopy or organic compounds.

The development of molecular electronics has become the mainstream of scientific research in recent decades. Applications include light-emitting diodes, solar cells, thin-film transistors, and sensors, among others. New-generation organic materials possess the virtues of softness, light weight, easy processing, design flexibility, and so on. This book focuses on the preparation of new functional organic materials. It includes a brief theoretical/kinetic discussion. The text lays special emphasis on the design of organic structures and the way they perform the designated functional properties. It will help organic chemists, particularly synthetic chemists, to light up their inspirations.

The derivation of structural information from spectroscopic data is now an integral part of 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 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) 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 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 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 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 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 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 31P, 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 Chemistry, Pharmacy, Biochemistry and those taking courses in Organic Chemistry. Also available: Instructors Guide and Solutions Manual to Organic Structures from 2D NMR Spectra

PRINCIPLES AND CHEMICAL APPLICATIONS FOR B.SC.(HONS) POST GRADUATE STUDENTS OF ALL INDIAN UNIVERSITIES AND COMPETITIVE EXAMINATIONS.

The text Organic Structures from 2D NMR Spectra contains a graded set of structural problems employing 2D-NMR spectroscopy. The Instructor's Guide and Solutions Manual to Organic Structures from 2D NMR Spectra is a set of step-by-step worked solutions to every problem in Organic Structures from 2D NMR Spectra. While it is absolutely clear that there are many ways to get to the correct solution of any of the problems, the instructor's guide contains at least one complete pathway to every one of the questions. In addition, the instructor's guide carefully rationalises every peak in every spectrum in relation to the correct structure. The Instructor's Guide and Solutions Manual to Organic Structures from 2D NMR Spectra: Is a complete set of worked solutions to the problems contained in Organic Structures from 2D NMR Spectra. Provides a step-by-step description of the process to derive structures from spectra as well as annotated 2D spectra indicating the origin of every cross peak. Highlights common artefacts and re-enforces the important characteristics of the most common techniques 2D NMR techniques - including COSY, NOESY, HMBC, TOCSY, CH-Correlation and multiplicity-edited C-H Correlation. This guide is an essential aid to those teachers, lecturers and instructors who use Organic Structures from 2D NMR as a text to teach students of Chemistry, Pharmacy, Biochemistry and those taking courses in Organic Chemistry. For more information on Organic Structures from 2D NMR Spectra Handbook of Infrared and Raman Spectra of Inorganic Compounds and Organic Salts

Although numerical data are, in principle, universal, the compilations presented in this book are extensively annotated and interleaved with text. This translation of the second German edition has been prepared to facilitate the use of this work, with all its valuable detail, by the large community of English-speaking scientists. Translation has also provided an opportunity to correct and revise the text, and to update the nomenclature. Fortunately, spectroscopic data and their relationship with structure do not change much with time so one can predict that this book will, for a long period of time, continue to be very useful to organic chemists involved in the identification of organic compounds or the elucidation of

their structure. Klaus Biemann Cambridge, MA, April 1983 Preface to the First German Edition Making use of the information provided by various spectroscopic tech niques has become a ·matter of routine for the analytically oriented organic chemist. Those who have graduated recently received extensive training in these techniques as part of the curriculum while their older colleagues learned to use these methods by necessity. One can, therefore, assume that chemists are well versed in the proper choice of the methods suitable for the solution of a particular problem and to translate the experimental data into structural information.

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

Organic Structure Determination Using 2-D NMR Spectroscopy: A Problem-Based Approach, Second Edition, is a primary text for a course in two-dimensional (2-D) nuclear magnetic resonance (NMR) techniques, with the goal to learn to identify organic molecular structure. It presents strategies for assigning resonances to known structures and for deducing structures of unknown organic molecules based on their NMR spectra. The book begins with a discussion of the NMR technique, while subsequent chapters cover instrumental considerations; data collection, processing, and plotting; chemical shifts; symmetry and topicity; through-bond effects; and through-space effects. The book also covers molecular dynamics; strategies for assigning resonances to atoms within a molecule; strategies for elucidating unknown molecular structures; simple and complex assignment problems; and simple and complex unknown problems. Each chapter includes problems that will enable readers to test their understanding of the material discussed. The book contains 30 known and 30 unknown structure determination problems. It also features a supporting website from which instructors can download the structures of the unknowns in selected chapters, digital versions of all figures, and raw data sets for processing. This book will stand as a single source to which instructors and students can go to obtain a comprehensive compendium of NMR problems of varying difficulty. Presents strategies for assigning resonances to known structures and for deducing structures of unknown organic molecules based on their NMR spectra Contains 30 known and 30 unknown structure determination problems Features a supporting website from which instructors can download the structures of the unknowns in selected chapters, digital versions of all figures, and raw data sets for processing

Taking a problem-based approach, the authors provide a practice-oriented and systematic introduction to both organic and inorganic structure determination by spectroscopic methods. This includes mass spectrometry, vibrational spectroscopies, UV/VIS spectroscopy and NMR as well as applying combinations of these methods. The authors show how to elucidate chemical structures with a minimal number of spectroscopic techniques. Readers can train their skills by more than 400 problems with varying degree of sophistication. Interactive Powerpoint-Charts are available as Extra Materials to support self-study.