

Spectroscopic Methods In Organic Chemistry

A unique textbook, aimed at undergraduate students, containing large numbers of spectra, problems and marginal notes, specifically chosen to highlight the points being discussed.

Originally published in 1962, this was the first book to explore the identification of organic compounds using spectroscopy. It provides a thorough introduction to the three areas of spectrometry most widely used in spectrometric identification: mass spectrometry, infrared spectrometry, and nuclear magnetic resonance spectrometry. A how-to, hands-on teaching manual with considerably expanded NMR coverage--NMR spectra can now be interpreted in exquisite detail. This book: Uses a problem-solving approach with extensive reference charts and tables. Offers an extensive set of real-data problems offers a challenge to the practicing chemist

Intended for advanced readers, this is a review of all relevant techniques for structure analysis in one handy volume. As such, it provides the latest knowledge on spectroscopic and related techniques for chemical structure analysis, such as NMR, optical spectroscopy, mass spectrometry and X-ray crystallography, including the scope and limitation of each method. As a result, readers not only become acquainted with the techniques, but also the advantages of the synergy between them. This enables them to choose the correct analytical method for each problem, saving both time and resources. Special emphasis is placed on NMR and its application to absolute configuration determination and the analysis of molecular interactions. Adopting a practical point of view, the author team from academia and industry guarantees both solid methodology and applications essential for structure determination, equipping experts as well as newcomers with the tools to solve any structural problem.

VCD Spectroscopy for Organic Chemists

Tables of Spectral Data for Structure Determination of Organic Compounds

An Introduction to Spectroscopic Methods in Organic Chemistry

Organic Spectroscopic Analysis

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This book provides a comprehensive review of the application of 17O NMR spectroscopy to organic chemistry. Topics include the theoretical aspects of chemical shift, quadrupolar and J coupling; 17O enrichment; the effect of steric interactions on 17O chemical shifts of functional groups in flexible and rigid systems; the application of 17O NMR spectroscopy to hydrogen bonding investigations; mechanistic problems in organic and bioorganic chemistry; and 17O NMR spectroscopy of oxygen monocoordinated to carbon in alcohols, ethers, and derivatives. Recent results that show correlations between molecular geometry, determined by X-ray studies and estimated by molecular mechanics calculations, and 17O chemical shifts are also covered. 17O Spectroscopy in Organic Chemistry provides important reference information for organic chemists and other scientists interested in 17O NMR spectroscopy as a tool for obtaining new structural and chemical data about organic molecules.

Clearly structured, easy to read and optimal to understand, this extensive compendium fills the gap between textbooks devoted to either spectra interpretation or basic physical principles. The original Chinese editions have already sold over 18,500 copies, and the material is taken from the latest literature from around the world, plus technical information provided by the manufacturers of spectroscopic instruments. Alongside basic methods, Professor Ning presents up-to-date developments in NMR, MS, IR and Raman spectroscopy, such as pulsed-field gradient technique, LC-NMR, and DOSY. He stresses the application of spectroscopic methods, interpreting them in great detail and depth since most of the selected spectra may be applied to practical work, as well as summarizing the rules for their interpretation. He also incorporates his original ideas, including a comparison of the common points in different spectroscopic techniques. This monograph features a unique structure, a typical example being the discussion of 2D NMR starting from pulse sequence units, which construct various pulse sequences for related 2D NMR. A complete chapter deals with the determination of configurations and conformations of organic compounds and even biological molecules from the viewpoint of spectroscopic methodologies, while one whole section is dedicated to the interpretation of mass spectra produced by soft ionization techniques. The principles of mass analyzers, especially the ion trap, are discussed in great depth, together with a concise summary of the MS fragmentation and rearrangement of common compounds, allowing readers to easily predict related mass spectrometric reactions. All the three kinds of library retrieval of mass spectra are presented in detail, together with recent developments in molecular vibration spectroscopy. The whole is rounded off with several appendices, including a subject index for rapid reference. With a foreword by the Nobel prizewinner, Richard R. Ernst.

Nuclear Magnetic Resonance and Infrared Spectroscopy

Computational Spectroscopy

Pearson New International Edition

Structural Analysis of Organic Compounds by Combined Application of Spectroscopic Methods

Table -- Combination tables -- 13C NMR spectroscopy -- 1H NMR spectroscopy -- IR spectroscopy -- Mass spectrometry -- UV/Vis spectroscopy.

An Introduction to Spectroscopic Methods for the Identification of Organic Compounds, Volume 2 covers the theoretical aspects and some applications of certain spectroscopic methods for organic compound identification. This book is composed of 10 chapters, and begins with an introduction to the structure determination from mass spectra. The subsequent chapter presents some mass spectrometry seminar problems and answers. This presentation is followed by discussions on the problems concerning the application of UV spectroscopy and electron spin resonance spectroscopy. Other chapters deal with some advances and development in NMR spectroscopy and the elucidation of structural formula of organic compounds by a combination of spectral methods. The final chapter surveys seminar problems and answers in the identification of organic compounds using NMR, IR, UV and mass spectroscopy. This book will prove useful to organic and analytical chemists.

An Introduction to Spectroscopic Methods for the Identification of Organic Compounds, Volume 1: Nuclear Magnetic Resonance and Infrared Spectroscopy discusses how spectral data can be translated into the structural formula of organic compounds and provides reference data and revised correlation tables for the initiated. The text describes high resolution nuclear magnetic resonance spectroscopy; the applications of nuclear magnetic resonance spectroscopy in organic chemistry; and correlation tables for nuclear magnetic resonance spectra. Nuclear magnetic resonance spectroscopy seminar problems and answers; the theoretical basis of infrared spectroscopy; and the applications of infrared spectroscopy to organic chemistry are also encompassed. The book further tackles infrared spectroscopic problems and answers, as well as correlation tables for infrared spectra.

Structure Elucidation in Organic Chemistry

The Search for the Right Tools

An Introduction to Spectroscopic Methods for the Identification of Organic Compounds

A Guide for Students of Organic Chemistry

E. Breitmaier, W. Voelter Carbon-13 NMR Spectroscopy High-Resolution Methods and Applications in Organic Chemistry and Biochemistry Third, completely revised edition New techniques and increased use of computers have led to rapid development in 13C NMR spectroscopy with enhanced instrumental sensitivity and improved quality of the spectra. This necessitated a complete revision when the third edition of this successful monograph was prepared. The new methods described include those for multiplicity analysis and two-dimensional homo- or hetero-nuclear shift correlations. As in the second edition, the authors survey the large number of 13C NMR applications to organic molecules and natural products in a representative and systematic rather than an exhaustive way. New sections about coupling constants, organophosphorus and organometallic compounds as well as synthetic polymers have been added. The scope remains limited to high-resolution methods and molecular systems.

Guide to Spectroscopic Identification of Organic Compounds is a practical "how-to" book with a general problem-solving algorithm for determining the structure of a molecule from complementary spectra or spectral data obtained from MS, IR, NMR, or UV spectrophotometers. Representative compounds are analyzed and examples are solved. Solutions are eclectic, ranging from simple and straightforward to complex. A picture of the relationship of structure to physical properties, as well as to spectral features, is provided. Compounds and their derivatives, structural isomers, straight-chain molecules, and aromatics illustrate predominant features exhibited by different functional groups. Practice problems are also included. Guide to Spectroscopic Identification of Organic Compounds is a helpful and convenient tool for the analyst in interpreting organic spectra. It may serve as a companion to any organic textbook or as a spectroscopy reference; its size allows practitioners to carry it along when other tools might be cumbersome or expensive.

This introductory text describes the uses of the 4 spectroscopic methods, UV, IR, NMR, and mass spectra in organic chemistry. New material includes extended coverage of 2-D NMR spectra and the introduction of the powerful techniques of TOCSY, ESI and MALDI.

Structure Determination of Organic Compounds

Circular Dichroism and Magnetic Circular Dichroism Spectroscopy for Organic Chemists

Structural Identification of Organic Compounds with Spectroscopic Techniques

Essential Practical NMR for Organic Chemistry

An understanding of spectroscopic techniques in the analysis of chemical structures is essential to all chemistry degree courses. This new addition to the Oxford Chemistry Primers series provides the essential material needed by undergraduates, in a compact form. It will be beneficial to postgraduates in organic chemistry as reference material in their daily research.

Structural Analysis of Organic Compounds covers some practical analytical aspects of organic structural analysis by combined application of spectroscopic methods. This book is composed of three parts encompassing 35 chapters that specifically describe infrared-, ultraviolet-, proton and carbon-13 nuclear magnetic resonance and mass spectroscopy. Considerable chapters discuss the problems intended to cover a wide variety of chemical structure and spectroscopic argument, thereby exemplifying interpretations and comment on specific practical aspects of the problem solving procedure. The remaining chapters provide short supplementing research concerning various aspects of structural analysis. This book will prove useful to organic and analytical chemists.

Download Area for Lecturers: www.thieme.de/specials/hmz_en.html This book provides the necessary equipment for the application of spectroscopic methods in organic chemistry, as required as part of chemistry courses in all universities. The following methods are explained and examples given: UV/Vis Spectroscopy, derivative Spectroscopy, chiroptical methods CD and ORD. Aggregated molecules, charge transfer complexes, conjugated oligomers. Infrared (IR) and Raman Spectroscopy, Fourier transform IR spectroscopy, and GC/IRcombination methods. Nuclear Magnetic Resonance Spectroscopy (NMR), 1H-, 13C-, 19F-, 15N- and 31P-NMR, spin decoupling, triple resonance, INDOOR difference spectroscopy, 2D- and 3D-NMR, COSY, TOCSY, ROESY and NOESY spectra, NOE, INEPT, and DEPT technique, DEPTQ, HETCOR, HRMAS, INADEQUATE and lanthanide shift reagents, simulation and calculation of spectra, and the combination of separation and NMR methods. The new 2D NMR techniques TOCSY, HMQC and HMBC, more examples and a guide to completely assign all 1H and 13C NMR signals of a given substrate. Mass spectrometry (MS), electron impact and chemical ionization (EI and CI), fast atom bombardment (FAB), electrospray and thermospray ionization (ESI and TSI), MS/MS technique (MSn), field ionization and field desorption (FI and FD), atmospheric pressure chemical ionization (APCI), MALDI TOF technique, GC/MS, LC/MS, and HPLC-UV(DAD)-APCI combination MS/MS technique. Fourier transform ion cyclotron resonance MS (FT-ICR-MS). The layout and many tables help to introduce the reader to spectroscopy. The extensive and thorough approach makes the text the first choice both as a companion for the professional chemists and as a refresher course in practical spectroscopy. The second English edition is a translation of the 7th German edition, in which several major alterations and didactic improvements have been made. For further information on our chemistry products, please visit: Thieme Chemistry.

Spectroscopic Methods in Organic Chemistry [by] Dudley H. Williams [and] Ian Fleming

High-Resolution Methods and Applications in Organic Chemistry and Biochemistry

Spectroscopic Techniques for Organic Chemists

Organic Spectroscopy

A knowledge of spectroscopic methods is required to interpret the shape and structure of compounds - this informative book concentrates on their application to inorganic compounds. The emphasis is placed on obtaining and interpreting the data rather than concentrating on the theory. To this end, examples are given in the text and worked through to show the processes involved in assigning spectra and obtaining information from them. This essential text for all undergraduate chemists will also benefit postgraduate students researching in the field of inorganic chemistry.

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. 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 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 resonance (NMR) spectroscopy; an introduction to biological molecules in mass spectrometry; and coverage of modern techniques alongside DEPT, COSY, and HECTOR. Important Notice: Media content referenced within the product description or the product text may not be available in the ebook version.

Introduction to Spectroscopic Structure Determination is a sophomore-level book with emphasis on structure problem solving. Taber has arranged the material in such a way that the students can work the problems and learn the procedures on their own, minimizing the time taken in lecture.

Spectroscopic Methods in Organic Chemistry

Organic Spectroscopic Structure Determination

Carbon-13 NMR Spectroscopy

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. 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. 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 nucleus is excited. 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. The book serves as an introductory textbook in the identification of organic compounds by spectroscopic means. Covers the usual techniques of infrared (IR), proton nuclear magnetic resonance (1H nmr) ultraviolet and mass spectroscopy with over 230 actual spectra and 100 worked-out problems. Covers the increasingly common techniques of carbon-13 nmr and Fourier transform nmr methods in a simple, non-mathematical way. Also discusses computer methods of iterating theoretical nmr spectra for a best fit with experimental data. Includes a CD-ROM with the LACON III program in a conversational timesharing version.

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 vocabulary, by the 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 corrections are few. The text 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 book by various spectroscopic techniques 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 them 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.

Tables of Spectral Data

Introduction to Spectroscopy

By Dudley H. Williams and Ian Fleming; Consulting Editor: P. Sykes

17 O NMR Spectroscopy in Organic Chemistry

Spectroscopic Methods in Organic ChemistrySpringer Nature

Download Area for Lecturers: www.thieme.de/specials/hmz_en.html This book provides the necessary equipment for the application of spectroscopic methods in organic chemistry, as required as part of chemistry courses in all universities. The following methods are explained and examples given: UV/Vis Spectroscopy, derivative Spectroscopy, chiroptical methods CD and ORD. Aggregated molecules, charge transfer complexes, conjugated oligomers. Infrared (IR) and Raman Spectroscopy, Fourier transform IR spectroscopy, and GC/IRcombination methods. Nuclear Magnetic Resonance Spectroscopy (NMR), 1H-, 13C-, 19F-, 15N- und 31P-NMR, spin decoupling, triple resonance, INDOOR difference spectroscopy, 2D- and 3D-NMR, COSY, TOCSY, ROESY and NOESY spectra, NOE, INEPT, and DEPT technique, DEPTQ, HETCOR, HRMAS, INADEQUATE and lanthanide shift reagents, simulation and calculation of spectra, and the combination of separation and NMR methods. The new 2D NMR techniques TOCSY, HMQC and HMBC, more examples and a guide to completely assign all 1H and 13C NMR signals of a given substrate. Mass spectrometry (MS), electron impact and chemical ionization (EI and CI), fast atom bombardment (FAB), electrospray and thermospray ionization (ESI and TSI), MS/MS technique (MSn), field ionization and field desorption (FI and FD), atmospheric pressure chemical ionization (APCI), MALDI TOF technique, GC/MS, LC/MS, and HPLC-UV(DAD)-APCI combination MS/MS technique. Fourier transform ion cyclotron resonance MS (FT-ICR-MS). The layout and many tables help to introduce the reader to spectroscopy. The extensive and thorough approach makes the text the first choice both as a companion for the professional chemists and as a refresher course in practical spectroscopy. The second English edition is a translation of the 7th German edition, in which several major alterations and didactic improvements have been made. For further information on our chemistry products, please visit: Thieme Chemistry.

Summarises the relationship between different types of spectra, describing qualitative and quantitative methods used to analyse CD and MCD spectral data.

Mass Spectrometry, Ultraviolet Spectroscopy, Electron Spin Resonance Spectroscopy, Nuclear Magnetic Resonance Spectroscopy (Recent Developments), Use of Various Spectral Methods Together, and Documentation of Molecular Spectra

Introduction to Organic Spectroscopy

Inorganic Spectroscopic Methods

Spectrometric Identification of Organic Compounds

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.

Stimulated by the increasing importance of chiral molecules as pharmaceuticals and the need for enantiomerically pure drugs, techniques in chiral chemistry have been expanded and refined, especially in the areas of chromatography, asymmetric synthesis, and spectroscopic methods for chiral molecule structural characterization. In addition to synthetic chiral molecules, naturally occurring molecules, which are invariably chiral and generally enantiomerically enriched, are of potential interest as leads for new drugs. VCD Spectroscopy for Organic Chemists discusses the applications of vibrational circular dichroism (VCD) spectroscopy to the structural characterization of chiral organic molecules. The book provides all of the information about VCD spectroscopy that an organic chemist needs in order to make use of the technique. The authors, experts responsible for much of the existing literature in this field, discuss the experimental measurement of VCD and the theoretical prediction of VCD. In addition, they evaluate the advantages and limitations of the technique in determining molecular structure. Given the availability of commercial VCD instrumentation and quantum chemistry software, it became possible in the late 1990s for chemists to use VCD in elucidating the stereochemistries of chiral organic molecules. This book helps organic chemists become more aware of the utility of VCD spectroscopy and provides them with sufficient knowledge to incorporate the technique into their own research.

A true introductory text for learning the spectroscopic techniques of Nuclear Magnetic Resonance, Infrared, Ultraviolet and Mass Spectrometry. It can be used in a stand alone spectroscopy course or as a supplement to the sophomore-level organic chemistry course.

Organic Structural Spectroscopy

Guide to Spectroscopic Identification of Organic Compounds

A Problem-based Learning Approach

Methods, Experiments and Applications

Boost your knowledge of modern spectroscopic methods! This reference work provides you with essential knowledge for the application of modern spectroscopic methods in organic chemistry. All methods are explained based on typical practical examples, theoretical aspects, and applications. The following spectroscopic methods are explained and examples are given: UV/Vis Spectroscopy Infrared (IR) and Raman Spectroscopy Nuclear Magnetic Resonance Spectroscopy (NMR) Mass Spectrometry (MS) The textbook has been a standard reference for decades. As it conveys necessary knowledge for examinations at all universities it is compulsory reading for every organic chemistry student!

Unique in its comprehensive coverage of not only theoretical methods but also applications in computational spectroscopy, this ready reference and handbook compiles the developments made over the last few years, from single molecule studies to the simulation of clusters and the solid state, from organic molecules to complex inorganic systems and from basic research to commercial applications in the area of environment relevance. In so doing, it covers a multitude of apparatus-driven technologies, starting with the common and traditional spectroscopic methods, more recent developments (THz), as well as rather unusual methodologies and systems, such as the prediction of parity violation, rare gas HI complexes or theoretical spectroscopy of the transition state. With its summarized results of so many different disciplines, this timely book will be of interest to newcomers to this hot topic while equally informing experts about developments in neighboring fields.

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 and 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.