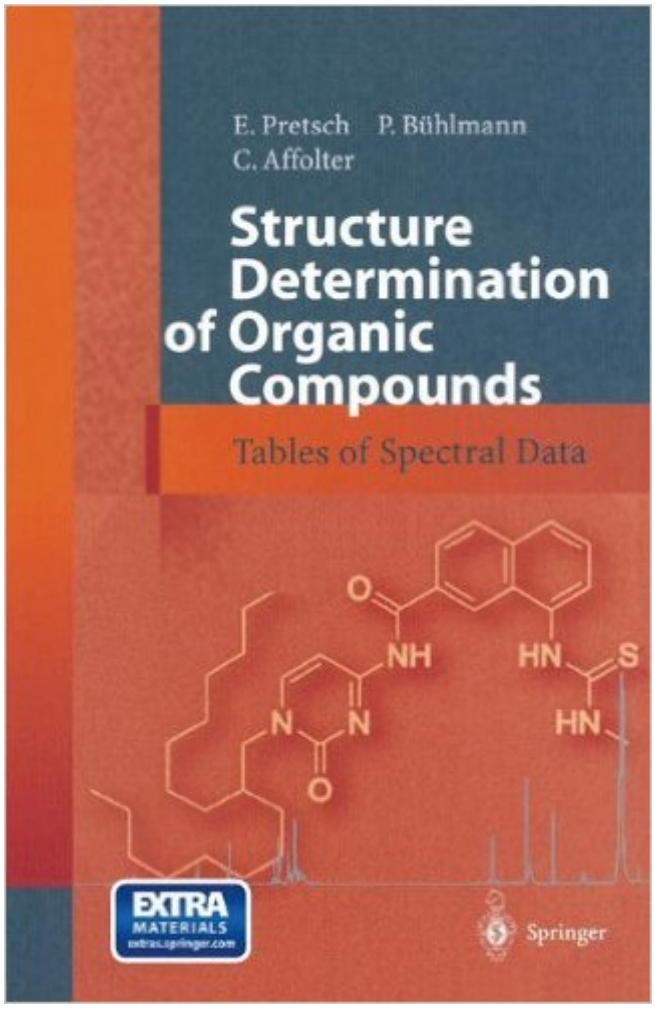
Structure Determination Of Organic Compounds: Tables Of Spectral Data



Synopsis

This volume presents in the form of texts, tables, charts and graphs a modern compilation of spectroscopic reference data for IR, UV/Vis, 1H- and 13C-NMR, MS (incl. prototype spectra of almost every important class of organic compounds and spectra of MALDI and FAB matrix materials) and is intended as a short textbook and a hands-on guide for interpreting experimental spectral data and elucidating the chemical structure of the respective compound behind it. The concise texts include special chapters on fragmentation rules in mass spectrometry and on currently used multipulse and 2-D NMR techniques. The book is primarily designed for students to be used during courses and exercises. The use of the book requires only basic knowledge of spectroscopic techniques, but is structured in such a way that it will support practitioners routinely faced with the task of interpreting such spectral information, and it will serve as data reference for specialists in the fields.

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Customer Reviews

The present data collection is intended to serve as an aid in the interpretation of molecular spectra for the elucidation and confirmation of the structure of organic compounds. It consists of reference data, spectra, and empirical correlations from 13C and 1H nuclear magnetic resonance (NMR), infrared (IR), mass, and ultraviolet-visible (UV/vis) spectroscopy. It is to be viewed as a supplement to textbooks and specific reference works dealing with these spectroscopic techniques. The use of

this book to interpret spectra only requires the knowledge of basic principles of the techniques, but its content is structured in a way that it will serve as a reference book also to specialists. Chapters 2 and 3 contain Summary Tables and combined tables of the most relevant spectral characteristics of structural elements. While Chapter 2 is organized according to the different spectroscopic techniques, Chapter 3 provides for each class of structural elements spectroscopic information obtained with various techniques. These two chapters should assist users that are less familiar with spectra interpretation to identify the classes of structural elements present in samples of their interest. The following four chapters cover data from 13C NMR, 1H NMR, IR, and mass spectroscopy, and are ordered exactly in the same manner by compound types. These cover the various skeletons (alkyl, alkenyl, alkynyl, alicyclic, aromatic, and heteroaromatic), the most important substituents (halogen, single-bonded oxygen, nitrogen, sulfur, and carbonyl), and some specific compound classes (miscellaneous compounds and natural products). Finally, a spectra collection of common solvents, auxiliary compounds (such as matrix materials and references) and commonly found impurities is provided for each method. Not only the strictly analogous order of the data but also the optical marks on the edge of the pages help fast cross-referencing between the various spectroscopic techniques. Although currently, UV/vis spectroscopy is only marginally relevant to structure elucidation, its importance might increase by the advent of high throughput analyses. Also, the reference data presented in Chapter 8 are useful in connection with optical sensors and the widely applied UV/vis detectors in chromatography and electrophoresis. Since a large part of the tabulated data either comes from our own measurements or is based on a large body of literature data, comprehensive references to published sources are generally not included. Whenever possible, the data refers to conventional modes and conditions of measurement. For example, unless the solvent is indicated, the NMR chemical shifts were determined usually with deuterochloroform or carbon tetrachloride as solvent. Likewise, the IR spectra were measured using solvents of low polarity, such as chloroform or carbon disulfide. Mass spectral data were recorded with electron impact ionization at 70 eV. While retaining the basic structure of the previous editions, numerous new entries have been added. Altogether, the amount of data has been more than doubled. The section on mass spectrometry (MS) is entirely new and contains a unique collection of fragmentation rules for the various compound classes. As a new feature, prototype IR spectra for each class of compounds schematically show the analytically relevant absorption bands. The Combination Tables of the earlier editions have been extended and arranged in two chapters, the first organized according to band positions and the second according to compound classes. The enclosed compact disc contains programs for estimating 13C and 1H chemical shifts of organic

compounds containing up to 15 non-hydrogen atoms. Both programs are available for Windows and Macintosh systems and require a Java environment for the graphical structure input. Technical details about the requirements and installation procedures are given in the corresponding ReadMe files. Extensive help files are available as part of the programs. In addition, the structure generator Assemble 2.0 (also limited to 15 non-hydrogen atoms) is available for Windows systems. Based on the molecular formula and available structural information, it is capable of generating all possible structural isomers. An extensive hypertext based tutorial describes its main features. It is especially recommended as a quality control tool to check if alternative solutions that also agree with the experimental data have gone unnoticed. [Why did I give 5 points: Because this book is absolutely unique in its form, and because the "not rated" option did not work, preventing me from being more modest.]

If you are taking a class in organic spectroscopy or use NMR all the time in your lab, then this book is a must. Gives you table after table of chemical shifts for C-13 NMR, H1-NMR, IR, Mass Spec, and UV/Vis. It also comes with a very useful NMR Predictor CD.

I’m taking an organic spectroscopy course for my graduate program in Organic chemistry and my exams consist of MS, IR, proton NMR, and C13 NMR spectra.This book is absolutely incredible. It gives you chemical shifts for nearly every conceivable structure for proton and C13 NMR and it also gives you absorptions for the IR frequencies of known functional groups. It has helped me many times in trying to determine the structure of an unknown compound.Like the other reviewer said, this book is the bible of organic spectroscopy. I see it being used all the time in the organic research lab when graduate students are trying to figure out what they synthesized.

I bought this book for a spectroscopy class I’m taking. I was worried that getting an earlier version would cause me to lose a lot of content, but really the only difference between this 3rd edition and the 4th is a chapter on heteroatom NMR, which you can easily get from someone else if others in your class get the updated version. The book is a fabulous reference for problem-solving, but doesn’t go into detail explaining the theory behind it or anything, so if you are looking for that, I’d recommend getting a textbook like the ones from Silverstein or Crews.

This is the best organic spectroscopy book I have ever found. If you have to take any kind of organic spec class, this is definitely a must.

I ordered this book because I was having a hard time evaluating NMR spectras I collected preparing my PhD thesis. The book contains an amazing amount of information in great detail. It supplies you with table data you can use to predict shifts of protons and carbons. It also contains many examples about natural products in general, sugars, DNA bases, cyclitols. I also found many details about IR spectra. I believe this book can be used by experienced scientists but it can also help students (both under and postgraduated) find their way through the maze of numbers and coupling costants.It is the best book I purchased up to now!Dr. Anastasia Varvogli

I find this reference to be greatly helpful. Bare in mind, that is a reference, not a textbook on organic spectroscopy, with little information on how to go about interpreting the various spectra. But nearly all the information one needs to interpret MS, UV/Vis, IR, and H and C NMR is in the book.My favorite feature are the combination spectra of common solvents. Much more helpful than simply peak data. I probably look at those pages more often than any others. I recommend this book, especially to newer organic chemists.

if you’re a synthetic chemist you need this booksaves you a ton of time not having to check a dozen different references, it’s all in one place

(Paperback)) Organic Perfume: The Ultimate Beginner's Guide to Making the Best Organic Perfume in 24 Hours or Less! Organic Manifesto: How Organic Food Can Heal Our Planet, Feed the World, and Keep Us Safe The Organic Farming Manual: A Comprehensive Guide to Starting and Running a Certified Organic Farm Microsoft Excel 2013 Data Analysis with Tables Quick Reference Guide (Cheat Sheet of Instructions, Tips & Shortcuts - Laminated Card) Mathematical Physics of Quantum Wires and Devices: From Spectral Resonances to Anderson Localization (Mathematics and Its Applications) Spectral Interpretation of Decision Diagrams Introduction to Hilbert Space: And the Theory of Spectral Multiplicity (AMS Chelsea Publishing) Electromagnetic and Optical Pulse Propagation 1: Spectral Representations in Temporally Dispersive Media (Springer Series in Optical Sciences) (v. 1) Data Science and Big Data Analytics: Discovering, Analyzing, Visualizing and Presenting Data Data Science for Business: What You Need to Know about Data Mining and Data-Analytic Thinking