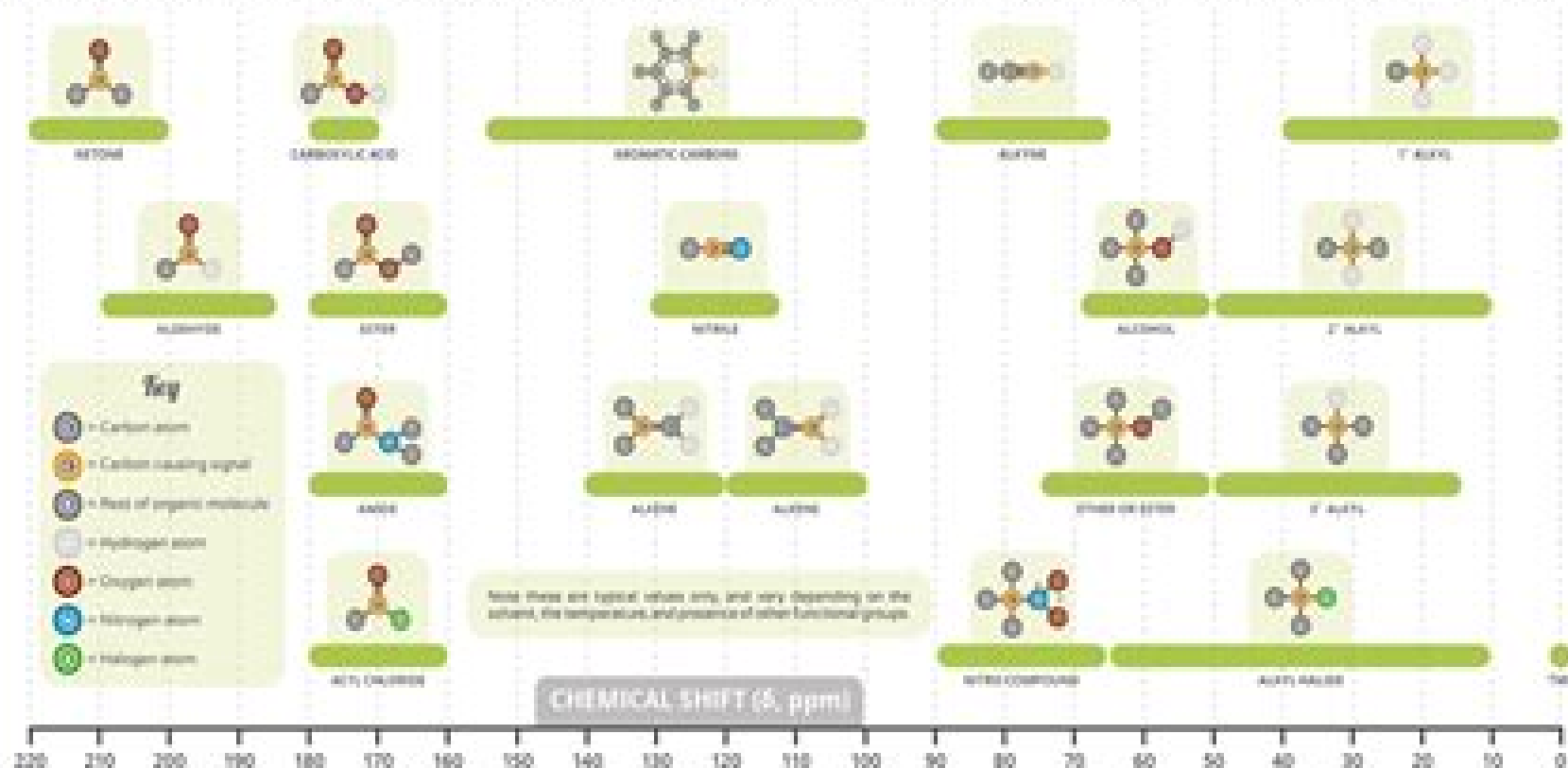


# A GUIDE TO $^{13}\text{C}$ NMR CHEMICAL SHIFT VALUES

Nuclear Magnetic Resonance (NMR) is a commonly used technique for organic compound structure determination. In  $^{13}\text{C}$  NMR, applying an external magnetic field causes the nuclei spin to flip. The environment of the carbon atom in the molecule affects where the signal is seen on the resultant spectrum.



$^{12}\text{C}$  99%

$^{13}\text{C}$  1%

Only 1% of carbon atoms are carbon-13, atoms which have one more neutron than carbon-12. NMR doesn't work for carbon-12, as its nucleus doesn't have a 'spin'. The frequency required to 'flip' a carbon-13 nucleus is around a quarter of that required to flip an hydrogen nucleus in  $^1\text{H}$ -NMR. As the probability of two adjacent carbons in a single molecule being carbon-13 atoms is very low, no splitting of peaks is seen, unlike in  $^1\text{H}$ -NMR.



# Nmr Spectroscopy Guide

**Thomas J. Bruno**



## **Nmr Spectroscopy Guide:**

*Analysis of NMR Spectra* R. A. Hoffman, S. Forsen, B. Gestblom, 2012-12-06 Nuclear magnetic resonance spectroscopy which has evolved only within the last 20 years has become one of the very important tools in chemistry and physics The literature on its theory and application has grown immensely and a comprehensive and adequate treatment of all branches by one author or even by several becomes increasingly difficult This series is planned to present articles written by experts working in various fields of nuclear magnetic resonance spectroscopy and will contain review articles as well as progress reports and original work Its main aim however is to fill a gap existing in literature by publishing articles written by specialists which take the reader from the introductory stage to the latest development in the field The editors are grateful to the authors for the time and effort spent in writing the articles and for their invaluable cooperation The Editors Analysis of NMR Spectra A Guide for Chemists R A HOFFMAN t S FORSEN Division of Physical Chemistry Chemical Center Lund Institute of Technology Lund Sweden B GESTBLOM Institute of Physics University of Uppsala Sweden Contents I Principles of NMR Spectroscopy 4 1 1 The Magnetic Resonance Phenomenon 4 a Nuclear Moments 4 b Magnetic Spin States and Energy Levels 5 c The Magnetic Resonance Condition 7 d The Larmor Precession 7 e Experimental Aspects 8 1 2 Chemical Shifts 9 a The Screening Constant 11 9 b Chemical Shift Scales 11 and r 10 1 3 Spin Coupling Constants 12 1 4 Intensities

**Modern NMR Spectroscopy** Jeremy K. M. Sanders, Brian K. Hunter, 1987 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 **50 and More Essential NMR Experiments** Matthias Findeisen, Stefan Berger, 2013-07-30 This book is the perfect link for learning how to perform the experiments after only having studied theory In eight chapters more than 50 essential NMR experiments are described in detail Special focus is put on the organic set of NMR spectra  $^1\text{H}$   $^{13}\text{C}$  APT COSY NOESY HSQC and HMBC Different chapters deal with advanced organic NMR selective methods heteronuclear NMR relaxation and diffusion measurements organic applications and maintenance Every experiment has a section providing the reader with the purpose and scope of the specific experiment Every experiment is concluded with the spectrum as it is obtained under the conditions described Questions and comments enable the reader to check their understanding The authors are very experienced and the whole book is in full color which enhances the reading experience and makes the spectra and other figures easier to understand This book is strongly recommended for all students and researchers who are involved in the structural elucidation of chemical compounds both in practical education and in pursuing research in particular if they handle an NMR spectrometer **Physico-chemical Applications of NMR** A. B. Kudryavtsev, W. Linert, 1996 The book is intended to help under and postgraduate students and young scientists in the correct application of NMR to the solution of physico chemical problems concerning the study of equilibria in solution The first part of the book Chapters 1 3 is a trivium but should enable a student to design and conduct

simple physico chemical NMR experiments The following chapters give illustrative material on the physico chemical applications of NMR of increasing complexity These chapters include the problem of determination of equilibrium and rate constants in solution the study of paramagnetism using NMR the application of Dynamic NMR techniques and relaxation measurements A multipurpose nonlinear regression program is supplied on disc for PC and is referred to throughout the book

*Principles of NMR Spectroscopy* David Goldenberg, 2016-03-31 With nearly 400 original illustrations this NMR primer provides an introduction to solution NMR spectroscopy at a level appropriate for advanced undergraduates graduate students and working scientists with backgrounds in chemistry or biochemistry With nearly 400 original illustrations this NMR primer provides an introduction to solution NMR spectroscopy at a level appropriate for advanced undergraduates graduate students and working scientists with backgrounds in chemistry or biochemistry It presents the underlying physics and mathematics in a way that is both accessible and sufficiently complete to allow a real understanding of modern multi dimensional experiments thereby giving readers the tools they need to move to more advanced textbooks and articles One special feature of this text is a thorough but accessible treatment of spin quantum mechanics including scalar coupled spins A novel style of vector diagram is used to represent the quantum correlations between coupled spins and the manipulation of these correlations by pulses and time evolution This will help to clarify what is arguably the most difficult aspect of NMR for students and practitioners to master

**Laboratory Guide to Proton NMR Spectroscopy** S. A. Richards, 1988-01-01

*Physician's Guide to the Diagnosis, Treatment, and Follow-Up of Inherited Metabolic Diseases* Nenad Blau, Marinus Duran, K Michael Gibson, Carlo Dionisi Vici, 2014-07-08 This book combining and updating two previous editions is a unique source of information on the diagnosis treatment and follow up of metabolic diseases The clinical and laboratory data characteristic of rare metabolic conditions can be bewildering for both clinicians and laboratory personnel Reference laboratory data are scattered and clinical descriptions may be obscure The Physician's Guide documents the features of more than five hundred conditions grouped according to type of disorder organ system affected e g liver kidney etc or phenotype e g neurological hepatic etc Relevant clinical findings are provided and pathological values for diagnostic metabolites highlighted Guidance on appropriate biochemical genetic testing is provided Established experimental therapeutic protocols are described with recommendations on follow up and monitoring The authors are acknowledged experts and the book will be a valuable desk reference for all who deal with inherited metabolic diseases

**Physician's Guide to the Laboratory Diagnosis of Metabolic Diseases** N. Blau, M. Duran, M.E. Blaskovics, K.M. Gibson, 2012-12-06 Delay and mistakes in the diagnosis of inherited metabolic diseases may have devastating consequences Reference laboratory data are scattered and clinical descriptions of rare conditions are hard to locate This book describes 298 disorders grouped into 35 chapters according to the type of condition Within each group of disorders chapters provide tables of pertinent clinical findings as well as reference and pathological values for crucial metabolites Relevant metabolic pathways and diagnostic flow charts are

included There are four indices to make the book as user friendly as possible Disorders index Signs and symptoms index Organs index and Tests index The Physician s Guide provides paediatricians and other physicians with a unique aid to help them select the correct diagnosis from a bewildering array of complex clinical and laboratory data

**Physico-chemical Applications Of Nmr: A Practical Guide** Andrei Borisovitch Koudriavtsev,A B Kudryavtsev,Wolfgang Linert,1996-09-20

The book is intended to help under and postgraduate students and young scientists in the correct application of NMR to the solution of physico chemical problems concerning the study of equilibria in solution The first part of the book Chapters 1 3 is a trivium but should enable a student to design and conduct simple physico chemical NMR experiments The following chapters give illustrative material on the physico chemical applications of NMR of increasing complexity These chapters include the problem of determination of equilibrium and rate constants in solution the study of paramagnetism using NMR the application of Dynamic NMR techniques and relaxation measurements A multipurpose nonlinear regression program is supplied on disc for PC and is referred to throughout the book

**Guide to Fluorine NMR for Organic Chemists** William R. Dolbier, Jr.,2016-08-22 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 **Handbook of Spectroscopy** G nter Gauglitz,Tuan

Vo-Dinh,2006-03-06 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

**Modern Methods in Solid-state NMR** Paul Hodgkinson,2018-04-09 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 **Handbook of**

**Spectroscopy** Günter Gauglitz, David S. Moore, 2014-06-09 This second thoroughly revised updated and enlarged edition 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 may be derived from spectra It also features new chapters on spectroscopy in nano dimensions nano optics and polymer analysis Clearly structured into sixteen sections it covers everything from spectroscopy in nanodimensions to medicinal applications spanning a wide range of the electromagnetic spectrum and the physical processes involved from nuclear phenomena to molecular rotation processes In addition data tables provide a comparison of different methods in a standardized form allowing readers to save valuable time in the decision process by avoiding wrong turns and also help in selecting the instrumentation and performing the experiments These four volumes are a must have companion for daily use in every lab NMR Spectroscopy Harald Günther, 2013-12-13

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 MODERN NMR SPECTROSCOPY: A GUIDE FOR CHEMISTS Jeremy K. M. Sanders, 1988 Handbook for the Analysis and Identification of

Alternative Refrigerants Thomas J. Bruno, 2019-07-23 Many laboratories are engaged in research on the development of new fluids for use as refrigerants to replace the fully halogenated materials that are believed to contribute to atmospheric ozone depletion. An integral part of this effort is the chemical analysis of new fluids that are synthesized, prepared and tested. This comprehensive book, which is divided into two parts, fills an important need in this vital chemical analysis protocol. The first part reviews the major chemical analysis methods that have been developed and used at NIST and in other laboratories. This review covers spectroscopic, chromatographic and wet analytical methods with treatment divided by qualitative identification, qualitative determinations and chemical reaction screening. The second part contains a compilation of analytical information of the new fluids and their products. Physical properties, mass spectra, infrared spectra, ultraviolet spectra, nuclear magnetic resonance spectra and gas chromatographic retention data are provided for each fluid or product.

Instructor's Guide and Solutions Manual to Organic Structures from 2D NMR Spectra, Instructor's Guide and Solutions Manual L. D. Field, A. M. Magill, H. L. Li, 2015-03-30 The text *Organic Structures from 2D NMR Spectra* contains a graded set of structural problems employing 2D NMR spectroscopy. The *Instructors 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 *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*. It 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.

**The Sadtler Guide to Carbon-13 NMR Spectra** Sadtler Research Laboratories, 1983      **A Guide to Materials Characterization and Chemical Analysis** John P. Sibilia, 1996-12-17 Diese sowohl für den Neuling als auch für den erfahrenen Wissenschaftler verfaßte Miniatur Enzyklopädie behandelt über 100 Untersuchungsmethoden zur Charakterisierung von Werkstoffen, von Bewertungen und chemischen Analysen bis zu physikalischen Verfahren. Der Autor beschreibt jede der Methoden nach Art und Weise ihres Einsatzes, der Probenvorbereitung und dem zugrundeliegenden wissenschaftlich-technischen Prinzip. Er bringt Anwendungsbeispiele aus dem akademischen und dem industriellen Bereich, um dem Leser eine Vorstellung von der Bedeutung dieser Techniken zu geben. Methoden zur Polymeranalyse mit Qualitäts-tests und Auswertungsverfahren sowie aus den Bereichen Oberflächenanalyse und Mikroskopie bilden unterstützt durch

anschauliche Abbildungen und Beispiele den Schwerpunkt des Buches      *Nuclear Magnetic Resonance Spectroscopy* Joseph B. Lambert, Eugene P. Mazzola, Clark D. Ridge, 2019-01-04 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



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