Chemical Shifts and Coupling Constants for Silicon-29. 2004-01-10 Nuclear Magnetic Resonance (NMR) is based on the fact that certain nuclei exhibit a magnetic moment, oriented by a magnetic field, and absorb characteristic frequencies in the radiofrequency part of the spectrum. The spectral lines of the nuclei are highly influenced by the chemical environment i.e. the structure and interaction of the molecules. NMR is now the leading technique and a powerful tool for the investigation of the structure and interaction of molecules. Volume III/35 “NMR-Data” is divided into several subvolumes and parts. Subvolume III/35A contains the nucleus 11B and 31P, subvolume III/35B contains the nuclei 19F and 15N, subvolume III/35C contains the nucleus 1H, subvolume III/35D contains the nucleus 13C, subvolume III/35E contains the nucleus 17O, and subvolume III/35F contains the nucleus 77Se. More nuclei will be presented later.

Chemical Shifts and Coupling Constants for Hydrogen-1. Fushimi Hiroki 2010-12-28 This volume includes several subvolumes and parts. Subvolume III/35A contains the nucleus 11B and 31P, subvolume III/35B contains the nuclei 19F and 15N, subvolume III/35C contains the nucleus 1H, subvolume III/35D contains the nucleus 13C, subvolume III/35E contains the nucleus 17O, and subvolume III/35F contains the nucleus 77Se. More nuclei will be presented later.


Chemical Shifts and Coupling Constants for Silicon-29. R. Gupta 2004-12-05 Nuclear Magnetic Resonance (NMR) is based on the fact that certain nuclei exhibit a magnetic moment, oriented by a magnetic field, and absorb characteristic frequencies in the radiofrequency part of the spectrum. The spectral lines of the nuclei are highly influenced by the chemical environment i.e. the structure and interaction of the molecules. NMR is now the leading technique and a powerful tool for the investigation of the structure and interaction of molecules. Volume III/35 “NMR-Data” is divided into several subvolumes and parts. Subvolume III/35A contains the nucleus 11B and 31P, subvolume III/35B contains the nuclei 19F and 15N, subvolume III/35C contains the nucleus 1H, subvolume III/35D contains the nucleus 13C, subvolume III/35E contains the nucleus 17O, and subvolume III/35F contains the nucleus 77Se. More nuclei will be presented later.

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Table of Spectral Data for Structure Determination of Organic Compounds. J. Petrich 2013-09-09 Nuclear Magnetic Resonance (NMR) spectroscopy has become the accepted method of choice for determining the structure of organic compounds. This table contains a list of organic compounds and their corresponding NMR spectral data including chemical shift values and coupling constants. However, the table does not represent all the organic compounds. Therefore, the reader should have a basic understanding of NMR spectroscopy and the interpretation of NMR spectra.

Guide to Fluorine NMR for Organic Chemists. W. R. Dolbier 2016-09-26 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 on nitrogen, silicon, and carbon; 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 nitrogens 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 offers 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

Oxygen-17 and Silicon-29. 2012-12-06 Although it was shown very early [1] that the isotope 29Si is very valuable for NMR research, severe technical difficulties had to be overcome before silicon spectra could be recorded. This was due to the low sensitivity of the isotope resulting from its low gyro magnetic ratio, its low relaxivity, and the low signal-to-noise ratio. The introduction of Fourier Transform technique (FT-NMR) helped to surmount most of these problems, with the result, that more and more papers concerning silicon NMR spectroscopy have been appearing. It seems now that silicon NMR spectroscopy is becoming an important technique for the study of silicon-containing compounds. The aims of this chapter are to present the basic concepts of the technique and to describe the experimental aspects of silicon NMR spectroscopy. The chapter covers a broad spectrum of topics related to the use of silicon NMR spectroscopy for the study of silicon-containing compounds, including the applications of silicon NMR spectroscopy to various fields such as analytical chemistry, materials science, and biochemistry.

CHEMICAL SHIFTS AND COUPLING CONSTANTS IN PENTAFUOROPHENYL DERIVATIVES. I. CORRELATIONS BETWEEN CHEMICAL SHIFTS AND COUPLING CONSTANTS. Guide to Fluorine NMR for Organic Chemists. W. R. Dolbier 2016-09-26 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 on nitrogen, silicon, and carbon; 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 nitrogens 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 offers 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

Annual Reports on NMR Spectroscopy. 1970-05-31 Annual Reports on NMR Spectroscopy

Chemical Shifts and Coupling Constants in Pentfluorophenyl Derivatives. II. Application to a Study of Bonding in Selected Compounds. M. Hofgren 1968 The π interactions within molecules containing the pentafluorophenyl group are highly influenced by the chemical environment i.e. the structure and interaction of the molecules. NMR is now the leading technique and a powerful tool for the investigation of the structure and interaction of molecules. Volume III/35 “NMR-Data” is divided into several subvolumes and parts. Subvolume III/35A contains the nucleus 11B and 31P, subvolume III/35B contains the nuclei 19F and 15N, subvolume III/35C contains the nucleus 1H, subvolume III/35D contains the nucleus 13C, subvolume III/35E contains the nucleus 17O, and subvolume III/35F contains the nucleus 77Se. More nuclei will be presented later.

Nuclear Magnetic Resonance—G. A Webb 2007-10-31 As a spectroscopic method, Nuclear Magnetic Resonance (NMR) has seen spectacular growth over the past two decades, both as a technique and in its applications. Today, the applications of NMR span a wide range of scientific disciplines, from physics to biology to medicine. Each volume of Nuclear Magnetic Resonance comprises a combination of annual and biennial reports which together provide comprehensive reviews of the literature on this topic. This Specialist Periodical Report reflects the growing volume of published work involving NMR techniques and applications, in particular NMR of natural macromolecules which is covered in two reports: “NMR of Proteins and Amino Acids” and “NMR of Carbohydrates, Lipids and Membranes”. For these wanting to become rapidly acquainted with specific areas of NMR, this title provides unrivalled scope of coverage. Seasoned practitioners of NMR will find this an invaluable source of current methods and applications. Specialist Periodical Reports provide systematic and detailed reviews and coverage in major areas of chemical research. Compiled by teams of leading authorities in the relevant subject areas, the series creates a unique service for the active research chemist, reviewer, in-depth accounts of progress in particular fields of chemistry. Subject coverage within different volumes of a given title is similar and publication is on an annual or biennial basis.

Chemical Shifts and Coupling Constants for Sulphur-33—Pushpa Paradies 2011 Chemical Shifts and Coupling Constants for Fluorine-19 and Nitrogen-15—1998-01-30 Nuclear magnetic resonance spectroscopy has proved invaluable for the investigation of the structure and of the intra- and inter-molecular interactions. Volume II of this series therefore provides a comprehensive and evaluated compilation of nuclear magnetic resonance data. Chemical shifts and coupling constants of boron-11 and phosphorus-31 (Subvol. A), Fluorine-19 and nitrogens-15 (Subvol. B), Hydrogen-1 (Subvol. C) and Carbon-13 (Subvol. D) compounds are tabulated together with the gross- and structure formulas and the most readily available solvents. Due to the large amount of data the chemical shifts are presented in the printed versions, and all the data, chemical shifts and coupling constants are provided on CD-ROM for Windows 3.x and Windows 95.

Structure Determination and Dynamics in Protein NMR—R. Gupta 2000-01-25 Volume 17 is the second in a series of periodic reports on protein NMR. Volume 16, with the subtitle Modern Techniques in Protein NMR, is the first in this series. These two volumes contain updated data on chemical shifts and coupling constants in proteins, and other structural and dynamical studies of proteins. Volume 17 contains major advances in: 1. Conformational Methods and II. Structure and Dynamics. The opening chapter of volume 17 gives a concise summary of the contents and the individual chapters present some of the recent, significant advances in the biomolecular NMR field with emphasis on the state of the art of 29Si NMR. NMR have been reviewed [1-4]. Although the theory of 29Si NMR is not yet understood because of the complexity and of the parameters, it promises to be of value mainly for two reasons: 1. Silicon is strategically located in the Periodic Table of the elements between the elements carbon, aluminum and phosphorus. For an unified theory of chemical shifts and coupling constants of the heavier elements silicon NMR values will be important. 2. The magnetic moment of silicon number is four. If the current view of the chemical shifts of the heavier elements is correct, then the paramagnetic part is dominant for the meanes shifted data. Two of the parameters used for the calculation of the paramagnetic part are bond orders and angles. Bond angles are rarely determined experimentally with high precision.

Aliphatic and Aromatic Hydrocarbons, Steroids, Carbohydrates—R. Gupta 2000-01-25 This volume presents comprehensive and evaluated compilation of nuclear magnetic resonance data. Chemical shifts and coupling constants of boron-11 and phosphorus-31 (Subvol. A), Fluorine-19 and nitrogens-15 (Subvol. B), Hydrogen-1 (Subvol. C) and Carbon-13 (Subvol. D) compounds are tabulated together with the gross- and structure formulas and the most readily available solvents. The temperature and the pH dependence, if reported in the original literature, is also indicated. Due to the large amount of data merely the chemical shifts are presented in the printed version, but all the data, chemical shifts and coupling constants are provided on the CD-ROM added to the printed volume. The present subvolume C, Part 1 provides the Chemical Shifts and Coupling Constants for Hydrogen-1 for Aliphatic and Aromatic Hydrocarbons, Steroids, and Carbohydrates.

Nuclear Magnetic Resonance Spectroscopy—Robin Kinsey Harris 1986 Nuclear Magnetic Resonance Spectroscopy explains the phenomenon from the point of view of a physical chemist interested in both fundamental principles and chemical applications. This rigorous but lucid text is highlighted by a large number of figures including illustrative spectra. Problems - with answers where appropriate - are also included. Table of contents: 1. The fundamentals; 2. Analysis of NMR spectra for isotropic solutions; 3. Relaxation and Fourier transform NMR; 4. Dipolar interactions and double resonance; 5. Chemical exchange and quadrupolar effects; 6. NMR of the solid state; 7. Special pulse sequences and two-dimensional NMR; 8. Chemical shifts and coupling constants. Appendices. Further reading. Answers to problems. Index.

Inorganic and Organometallic Compounds—R. Gupta 2001-01-26 The chemical shifts (δ ppm) and the structure formulas are given along with the complete references. The data are arranged according to the atomic number, and within a group, the data are arranged alphabetically according to the name of the element. The names of the compounds are written in the standard IUPAC nomenclature. The book is divided into three parts: 1. Oxigen-17 and Silicon-29, 2. Transition and inner Transition Elements, and 3. Noble Gases and other Elements. The chemical shifts δ (in ppm) and the structure formulas are given along with the complete references. The data are arranged according to the atomic number, and within a group, the data are arranged alphabetically according to the name of the element. The names of the compounds are written in the standard IUPAC nomenclature.

Spectroscopy—Peter M. Siral 2012-10-05 This book provides a novel view of spectroscopic methods: it describes spectroscopy holistically in terms of integral physical aspects instead of the classical methods: order acquisition and order interpretation. The order in spectroscopy is a reflection of resonance. These methods and their common physical basis, namely the reversible absorption of energy from the respective regions of the electromagnetic spectrum, are illustrated in a comprehensive manner with the help of a multitude of explicative color graphs.

Nuclear Magnetic Resonance of Biological Macromolecules—2001-07-12 This volume and its companion, Volume 338, supplement Volume 176, 177, 239, and 261. Chapters are written with a "hands-on" perspective. That is, practical applications with critical evaluations of methodological and experimental considerations needed to design, execute, and interpret NMR experiments pertinent to biological molecules.

13N-NMR Spectroscopy—C. Martin 2013-12-06 After the proton and carbon, nitrogen is, with oxygen, the most important atom in organic and especially biorganic macromolecules. However, the development of nitrogen spectroscopy is of a different character. This is recently due to the fact that nitrogen 14, which is the naturally abundant isotope, suffers, for structural studies, from the disadvantages inherent in nuclei with a quadrupolar moment (Table 1.1). Actually, indirect 15N measurements were reported in the early days of double resonance spectroscopy and the first direct detection of 15N resonance signals at the natural abundance level was achieved in 1964 (R. J. 1973-358 4.33 MHz (~ 17) using a 15 n.m. c.d. in the field sweep mode (~ 16.5 m). Signal-to-noise ratios only of 3.4 were obtained for neat liquids and this low sensitivity of the 15N resonance still remains the main disadvantage for 13C spectroscopy (Table 1.1). However, nitrogen-15 is, probably, no more than any other nucleus, benefited from the advances of NMR technology, i.e., Fourier transformation, multichannel facilities, wide-band super conducting solenoids, and, with the new generation of spectrometers, 15N-NMR is entering the field of routine investigation. Nevertheless, in spite of these spectacular improvements, obtaining 15N spectra of diluted species or large biochemical molecules is often not very easy and a good knowledge of the relaxation properties plays an important role in order to obtain the necessary signal to noise ratio to give good spectra. 15N can be considered as the natural choice for NMR spectroscopy in most cases, particularly in proteins, in which 13C is replaced by 15N in order to facilitate the interpretation of the resonances. This is especially the case for proteins that have a high proportion of aromatic residues. The most usual advantage is the fact that the 15N chemical shift is less influenced by the environment than the 13C one. 15N is also more susceptible to static and dynamic nuclear polarization, which can increase the sensitivity of the signal by a factor of 5 to 100.

Chemical Shifts and Coupling Constants for Hydrogen-1—Hilman R. Gupta 2000-01-25 Handbook of NMR Spectral Parameters 1979 (1979-01-30) As a spectroscopic method, Nuclear Magnetic Resonance (NMR) has seen spectacular growth over the past two decades, both as a technique and in its applications. Today, the applications of NMR span a wide range of scientific disciplines, from physics to biology to medicine. Each volume of Nuclear Magnetic Resonance comprises a combination of annual and biennial reports which together provide comprehensive coverage of the literature on this topic. This Specialist Periodical Report reflects the growing volume of published work involving NMR techniques and applications, in particular NMR of Natural macromolecules, which is covered in two reports: “NMR of Proteins and Amino Acids” and “NMR of Carbohydrates, Lipids and Membranes”. For these wanting to become rapidly acquainted with specific areas of NMR, this title provides unrivalled scope of coverage. Seasoned practitioners of NMR will find this an invaluable source of current methods and applications.