

NMR

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Editors: P. Diehl E. Fluck R. Kosfeld

Volume 7

C. W. Hilbers and C. MacLean

NMR of Molecules Oriented in Electric Fields

H. Pfeifer

**Nuclear Magnetic Resonance and Relaxation
of Molecules Adsorbed on Solids**



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NMR, 1972 **NMR Basic Principles and Progress / NMR Grundlagen und Fortschritte** P. Diehl, E. Flück, R. Kosfeld, 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 Contents c W Hilbers and C MacLean **NMR of Molecules Oriented in Electric Fields** **NMR Basic Principles and Progress. Grundlagen und Fortschritte** P. Diehl, C. L. Khetrapal, R. G. Jones, 2013-04-17 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 Contents P Diehl and C L Khetrapal **NMR Studies of Molecules Oriented in the Nematic Phase of Liquid Crystals** 1 R G Jones The Use of Symmetry in Nuclear Magnetic Resonance 97 **NMR Studies of Molecules Oriented in the Nematic Phase of Liquid Crystals** P DIEHL and C L KHETRAPAL Department of Physics University of Basel Switzerland Contents 1 Introduction 3 2 Liquid Crystals 4 2 1 Classification of Liquid Crystal Phases 4 2 2 Theories of the Liquid Crystalline State 5 2 3 Nematic Phases 6 3 Experimental 7 1 4 Basic Theory for I I 7 **NMR**, 1971 **NMR**, 1970 **Acta Physica Polonica**, 1973 Section A includes general physics solid state physics applied physics **NMR**, 1972 **Ab Initio Calculations** Petr Carsky, Miroslav Urban, 2012-12-06 Until recently quantum chemical ab initio calculations were restricted to atoms and very small molecules As late as in 1960 Allen and Karo stated Almost all of our ab initio experience derives from diatomic LCAO calculations Now we have found in the literature approximately eighty calculations three fourths of which are for diatomic molecules There are approximately twenty ab initio calculations for molecules with more than two atoms but there is a decided dividing line between the existing diatomic and polyatomic wave functions Confidence in the satisfactory evaluation of the many center two electron integrals is very much less than for the

diatomic case Among the noted twenty calculations SiH was the largest 4 molecule treated In most cases a minimal basis set was used and the many center two electron integrals were calculated in an approximate way Under these circumstances the ab initio calculations could hardly provide useful chemical information It is therefore no wonder that the dominating role in the field of chemical applications was played by semiempirical and empirical methods The situation changed essentially in the next decade The problem of many center integrals was solved efficient and sophisticated computer programs were developed basis sets suitable for a given type of problem were suggested and meanwhile a considerable amount of results has been accumulated which serve as a valuable comparative material The progress was of course inseparable from the development and availability of computers

N[uclear] M[agnetic] R[esonance], 1970 *Chemically Induced Dynamic Nuclear and Electron Polarizations-CIDNP and CIDEP* C. Richard, P. Granger, 2012-12-06 Anomalous electron spin state populations in the Electron Paramagnetic Resonance EPR spectra of radicals formed during radiolysis experiments were observed in 1963 by FESSENDEN and SCHULER 170a This phenomenon did not receive much attention at the time In 1967 BARGON FISCHER and JOHNSON 5 and independently WARD and LAWLOR 7 8 reported a similar phenomenon for Nuclear Magnetic Resonance NMR spectra taken during radical reactions emission or enhanced absorption or both The earliest attempts to explain this new NMR phenomenon treated these effects in a way similar to that of Dynamic Nuclear Polarization DNP or the Overhauser effect Although the polarization has a completely different origin DNP gave its name to this effect Chemically Induced Dynamic Nuclear Polarization CIDNP The name Chemically Induced Dynamic Electron Polarization CIDEP was introduced later by analogy with CIDNP After the initial publications all the new data demonstrated that the first theory could not be correct In 1969 a new theory was proposed by CLOSS 18 and independently by KAPTEIN and OOSTERHOFF 23 and called the radical pair theory This mechanism was proposed to account for the observations of polarization in both NMR and EPR The radical pair theory is based on weak interactions in a pair of radicals the strength of interaction between the electronic states of the radicals depends in particular on the nuclear spin states

NMR Basic Principles and Progress. Grundlagen und Fortschritte P. Diehl, C. L. Khetrpal, R. G. Jones, 2014-03-12 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 Contents P Diehl and C L Khetrpal NMR Studies of Molecules Oriented in the Nematic Phase of Liquid Crystals

1 R G Jones The Use of Symmetry in Nuclear Magnetic Resonance 97 NMR Studies of Molecules Oriented in the Nematic Phase of Liquid Crystals P DIEHL and C L KHETRAPAL Department of Physics University of Basel Switzerland Contents 1 Introduction 3 2 Liquid Crystals 4 2 1 Classification of Liquid Crystal Phases 4 2 2 Theories of the Liquid Crystalline State 5 2 3 Nematic Phases 6 3 Experimental 7 1 4 Basic Theory for I I 7 NMR Crystallography Robin K. Harris, Roderick E. Wasylishen, Melinda J. Duer, 2012-12-19 The content of this volume has been added to eMagRes formerly Encyclopedia of Magnetic Resonance the ultimate online resource for NMR and MRI The term NMR Crystallography has only recently come into common usage and even now causes raised eyebrows within some parts of the diffraction community The power of solid state NMR to give crystallographic information has considerably increased since the CPMAS suite of techniques was introduced in 1976 In the first years of the 21st century the ability of NMR to provide information to support and facilitate the analysis of single crystal and powder diffraction patterns has become widely accepted Indeed NMR can now be used to refine diffraction results and in favorable cases to solve crystal structures with minimal or even no diffraction data The increasing ability to relate chemical shifts including the tensor components to the crystallographic location of relevant atoms in the unit cell via computational methods has added significantly to the practice of NMR crystallography Diffraction experts will increasingly welcome NMR as an allied technique in their structural analyses Indeed it may be that in the future crystal structures will be determined by simultaneously fitting diffraction patterns and NMR spectra This Handbook is organised into six sections The first contains an overview and some articles on fundamental NMR topics followed by a section concentrating on chemical shifts and one on coupling interactions The fourth section contains articles describing how NMR results relate to fundamental crystallography concepts and to diffraction methods The fifth section concerns specific aspects of structure such as hydrogen bonding Finally four articles in the sixth section give applications of NMR crystallography to structural biology organic pharmaceutical chemistry inorganic materials chemistry and geochemistry About EMR Handbooks eMagRes Handbooks The Encyclopedia of Magnetic Resonance up to 2012 and eMagRes from 2013 onward publish a wide range of online articles on all aspects of magnetic resonance in physics chemistry biology and medicine The existence of this large number of articles written by experts in various fields is enabling the publication of a series of EMR Handbooks eMagRes Handbooks on specific areas of NMR and MRI The chapters of each of these handbooks will comprise a carefully chosen selection of articles from eMagRes In consultation with the eMagRes Editorial Board the EMR Handbooks eMagRes Handbooks are coherently planned in advance by specially selected Editors and new articles are written together with updates of some already existing articles to give appropriate complete coverage The handbooks are intended to be of value and interest to research students postdoctoral fellows and other researchers learning about the scientific area in question and undertaking relevant experiments whether in academia or industry Have the content of this Handbook and the complete content of eMagRes at your fingertips Visit www.wileyonlinelibrary.com/ref/eMagRes View other eMagRes publications here

Annales Societatis Chimicae Polonorum ,1973 ¹⁵N-NMR Spectroscopy G.J. Martin,M.L. Martin,J.-P.

Gouesnard,2012-12-06 After the proton and carbon nitrogen is with oxygen the most important atom in organic and especially bioorganic molecules However the development of nitrogen spectroscopy is indeed very recent This is 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 realized in 1964 R 17 at 4.33 MHz 1.1T using a 15 mm o.d. cell in the field sweep mode 0.16 min 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 ¹⁵N spectroscopy Table 1.1 However nitrogen 15 has probably more than any other nucleus benefited from the advances of NMR technology i.e. Fourier transformation multinuclear facilities wide bore superconducting 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 peculiar to ¹⁵N may be necessary in order to adjust the pulse sequences and the decoupler duty cycle correctly Section 2 Solid State NMR Studies of Biopolymers Anne E. McDermott,Tatyana Polenova,2012-12-19 The content of this volume has been added to eMagRes formerly Encyclopedia of Magnetic Resonance the ultimate online resource for NMR and MRI The field of solid state NMR of biological samples ssNMR has blossomed in the past 5-10 years and a cohesive overview of the technology is needed for new practitioners in industry and academia This title provides an overview of Solid State NMR methods for studying structure dynamics and ligand binding in biopolymers and offers an overview of RF pulse sequences for various applications including not only a systematic catalog but also a discussion of theoretical tools for analysis of pulse sequences Practical examples of biochemical applications are included along with a detailed discussion of the many aspects of sample preparation and handling that make spectroscopy on solid proteins successful About EMR Handbooks eMagRes Handbooks The Encyclopedia of Magnetic Resonance up to 2012 and eMagRes from 2013 onward publish a wide range of online articles on all aspects of magnetic resonance in physics chemistry biology and medicine The existence of this large number of articles written by experts in various fields is enabling the publication of a series of EMR Handbooks eMagRes Handbooks on specific areas of NMR and MRI The chapters of each of these handbooks will comprise a carefully chosen selection of articles from eMagRes In consultation with the eMagRes Editorial Board the EMR Handbooks eMagRes Handbooks are coherently planned in advance by specially selected Editors and new articles are written together with updates of some already existing articles to give appropriate complete coverage The handbooks are intended to be of value and interest to research students postdoctoral fellows and other researchers learning about the scientific area in question and undertaking relevant experiments whether in academia or industry Have

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High Resolution NMR Spectroscopy in Solids M.

Mehring, 2012-12-06 Manipulation and Dilution Tools for Ruling Abundant Species NMR is dead was the slogan heard in the late 1960s at least among physicists until John S Waugh and his co workers initiated a series of new NMR experiments which employed the coherent modulation of interactions by strong radiofrequency fields A wealth of new phenomena was observed which are summarized in the introduction for the convenience of the unbiased reader whereas Section 2 collects the basic spin interactions observed in solids Line narrowing effects in dipolar coupled solids by the application of multiple pulse experiments are extensively discussed in Section 3 Numerous extensions of the basic Waugh Huber and Haeberlen experiment have been developed by different groups and have been applied to the nuclei ^1H ^9Be ^{19}F ^{27}Al ^{31}P ^{63}Cu in solids Application of this technique to a variety of systems is still in progress and should reveal interesting insights into weak spin interactions in solids It was soon realized that rare spins could be used as monitors for molecular fields in the solid state however rare spin observation is difficult because of the small signal to noise ratio Pines Gibby and Waugh introduced a new concept of cross polarization based on ideas of Hahn and co workers which allows the detection of rare spins with increased sensitivity The dynamics involved are treated in detail Other sections merely list results obtained by the techniques described and demonstrate their usefulness in the investigation of dynamical problems in molecular and solid state physics *Catalog of Copyright Entries. Third Series* Library of Congress. Copyright Office, 1972 **Minnesota Union List of Serials**, 1974

Liquid Crystals Horst Stegemeyer, 2013-03-14 In 1959 about 1400 compounds forming liquid crystalline phases were known by 1992 this number had increased to about 50 000 In portable devices like wristwatches pocket calculators measuring instruments and laptop computers the liquid crystal display technology has gained total acceptance and is on the way to encompass the market of colour TV screens This development makes a volume devoted to liquid crystals in the series Topics in Physical Chemistry desirable Following the concept of this series an easy introduction to liquid crystals is given enabling the reader to understand the basic problems of liquid crystals research and application Because of the widespread field of different research activities in liquid crystals and applications various competent authors have been involved in writing chapters on Phase types structures and chemistry of liquid crystals Thermodynamical behavior and physical properties of thermotropic liquid crystals Liquid crystalline polymers Lyotropic liquid crystals Application of liquid crystals in spectroscopy Application of liquid crystals in display technology *Oxygen-17 and Silicon-29*, 2012-12-06 Although it was shown very early that the isotope ^{29}Si 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 gyromagnetic ratio its low abundance and the rather long relaxation times The introduction of the Fourier Transform Technique FT NMR helped to surmount most of these problems with the result that more and more papers concerning silicon NMR

appear. Thus it seems now that most of the salient features of ^{29}Si NMR are known today. Some resume of the state of the art of ^{29}Si NMR have been reported [1-4]. Although the theory of ^{29}Si NMR is not yet understood beyond the basic features 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 normal coordination number of silicon is four. If the current view of the chemical shifts of the heavier elements is correct, then the paramagnetic part is dominant for the measured shift 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.

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