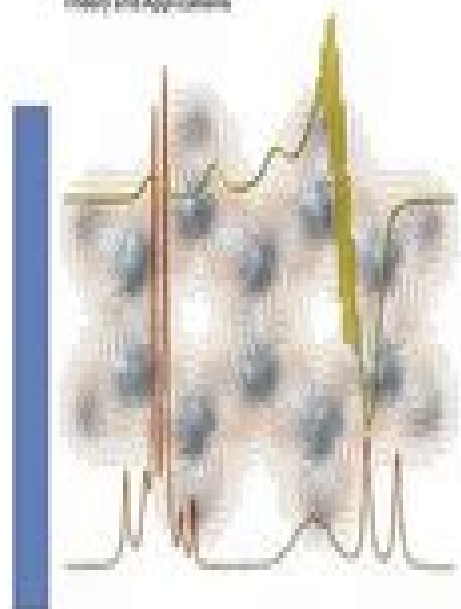


Edited by Martin Kaupp,
Michael Buhl, Vladimir G. Malkin

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Calculation of NMR and EPR Parameters

Theory and Applications



Calculation Of Nmr And Epr Parameters Theory And Applications

Marcel A. Müller



Calculation Of Nmr And Epr Parameters Theory And Applications:

Calculation of NMR and EPR Parameters Martin Kaupp, Michael Bühl, Vladimir G. Malkin, 2006-03-06 This is the first book to present the necessary quantum chemical methods for both resonance types in one handy volume emphasizing the crucial interrelation between NMR and EPR parameters from a computational and theoretical point of view Here readers are given a broad overview of all the pertinent topics such as basic theory methodic considerations benchmark results and applications for both spectroscopy methods in such fields as biochemistry bioinorganic chemistry as well as with different substance classes including fullerenes zeolites and transition metal compounds The chapters have been written by leading experts in a given area but with a wider audience in mind The result is the standard reference on the topic serving as a guide to the best computational methods for any given problem and is thus an indispensable tool for scientists using quantum chemical calculations of NMR and EPR parameters A must have for all chemists physicists biologists and materials scientists who wish to augment their research by quantum chemical calculations of magnetic resonance data but who are not necessarily specialists in these methods or their applications Furthermore specialists in one of the subdomains of this wide field will be grateful to find here an overview of what lies beyond their own area of focus

Principles and Applications of Density Functional Theory in Inorganic Chemistry I Nikolas Kaltsoyannis, John E. McGrady, 2004-09-14 It is difficult to overestimate the impact that density functional theory has had on computational quantum chemistry over the last two decades Indeed this period has seen it grow from little more than a theoretical curiosity to become a central tool in the computational chemist's armoury Arguably no area of chemistry has benefited more from the meteoric rise in density functional theory than inorganic chemistry the ability to obtain reliable results in feasible time scales on systems containing heavy elements such as the d and f transition metals has led to an enormous growth in computational inorganic chemistry The inorganic chemical literature reflects this growth it is almost impossible to open a modern inorganic chemistry journal without finding several papers devoted exclusively or in part to density functional theory calculations The real importance of the rise in density functional theory in inorganic chemistry is undoubtedly the much closer synergy between theory and experiment than was previously possible In these volumes world leading researchers describe recent developments in the density functional theory and its applications in modern inorganic and bioinorganic chemistry These articles address key issues in both solid state and molecular inorganic chemistry such as spectroscopy mechanisms catalysis bonding and magnetism The articles in volume I are more focussed on advances in density functional methodology while those in Volume II deal more with applications although this is by no means a rigid distinction

NMR Spectroscopic Parameters Gustavo Adolfo Aucar, 2025-07-30 NMR spectroscopy is one of the most useful tools to get reliable information about both the geometrical and the electronic structures of small size containing a few atoms to large size containing thousands of atoms molecules It can also give information about subtle and intrinsic characteristics of those molecules or chemical processes in which the

nuclei that resonate by NMR are involved To get this information requires both the computation and theoretical analysis of the spectroscopic parameters This book provides a basic presentation which is as thorough as possible of the most commonly used theories and models for the theoretical understanding and calculation of the spectroscopic parameters of NMR spectroscopy This information is combined with their applications in both model systems and complex systems the analysis of a few of the newest effects together with highly accurate calculations for small size molecules and their calculations in large sized compounds ionic liquids heavy atom containing systems lanthanide and actinide systems and solid state quantum systems The authors have been encouraged to present the most insightful ideas and the most important findings that one can get from NMR spectroscopy as well as its limitations or drawbacks This book is aimed at undergraduate and graduate students specialists and possibly industry workers who will find information about the theoretical developments that have been performed in the last decade enabling them to achieve highly accurate calculations and understandings that were not available previously The book also offers clarity in the exposition of abstract concepts that are not usually communicated together with simple and complex applications *Annual Reports on NMR Spectroscopy* Graham A. Webb, 2007-05-09

Nuclear magnetic resonance NMR is an analytical tool used by chemists and physicists to study the structure and dynamics of molecules In recent years no other technique has grown to such importance as NMR spectroscopy It is used in all branches of science where precise structural determination is required and where the nature of interactions and reactions in solution is being studied *Annual Reports on NMR Spectroscopy* has established itself as a premier means for the specialist and nonspecialist alike to become familiar with new techniques and applications of NMR spectroscopy Provides updates on the latest developments in NMR spectroscopy Includes comprehensive review articles Highlights the increasing importance of NMR spectroscopy as a technique for structural determination *High Resolution NMR Spectroscopy: Understanding Molecules and their Electronic Structures*, 2013-06-08 The progress in nuclear magnetic resonance NMR spectroscopy that took place during the last several decades is observed in both experimental capabilities and theoretical approaches to study the spectral parameters The scope of NMR spectroscopy for studying a large series of molecular problems has notably broadened However at the same time it requires specialists to fully use its potentialities This is a notorious problem and it is reflected in the current literature where this spectroscopy is typically only used in a routine way Also it is seldom used in several disciplines in which it could be a powerful tool to study many problems The main aim of this book is to try to help reverse these trends This book is divided in three parts dealing with 1 high resolution NMR parameters 2 methods for understanding high resolution NMR parameters and 3 some experimental aspects of high resolution NMR parameters for studying molecular structures Each part is divided into chapters written by different specialists who use different methodologies in their work In turn each chapter is divided into sections Some features of the different sections are highlighted it is expected that part of the readership will be interested only in the basic aspects of some chapters while other

readers will be interested in deepening their understanding of the subject dealt with in them Shows how NMR parameters are useful for structure assignment as well as to obtain insight on electronic structures Emphasis on conceptual aspects Contributions by specialists who use the discussed methodologies in their everyday work *Handbook of Solid State Chemistry, 6 Volume Set* Richard Dronskowski, Shinichi Kikkawa, Andreas Stein, 2017-10-23 This most comprehensive and unrivaled compendium in the field provides an up to date account of the chemistry of solids nanoparticles and hybrid materials Following a valuable introductory chapter reviewing important synthesis techniques the handbook presents a series of contributions by about 150 international leading experts the Who's Who of solid state science Clearly structured in six volumes it collates the knowledge available on solid state chemistry starting from the synthesis and modern methods of structure determination Understanding and measuring the physical properties of bulk solids and the theoretical basis of modern computational treatments of solids are given ample space as are such modern trends as nanoparticles surface properties and heterogeneous catalysis Emphasis is placed throughout not only on the design and structure of solids but also on practical applications of these novel materials in real chemical situations **High Resolution NMR Spectroscopy** Juha Vaara, 2013-06-08 The theory and quantum chemical calculations of the spectral parameters of nuclear magnetic resonance NMR are well established in the case of diamagnetic closed shell molecules In contrast NMR calculations of paramagnetic open shell molecules pNMR are scarce limited by both assumptions within the underlying theoretical background as well as the availability of computational implementations We discuss the systematic development of pNMR theory that recently culminated in a novel general and systematic electronic structure approach for the shielding tensor and the associated chemical shift for paramagnetic open shell atoms molecules and nonmetallic solids The approach has now been extended for the first time to a higher than doublet spin state as well as arbitrary spatial symmetry The approach is formulated without reference to spin susceptibility in contrast to the contemporary experimental procedure and approximate quantum chemical treatment of axial zero field splitting As a result of the systematic procedure all the temperature dependent hyperfine shielding terms are generalized and for example the leading order nonrelativistic dipolar term now provides an isotropic chemical shift contribution for species with triplet and higher spin multiplicity Recent first principles quantum chemical calculations of pNMR chemical shifts are reviewed both using the novel theory as well as earlier approaches *Spin States in Biochemistry and Inorganic Chemistry* Marcel Swart, Miquel Costas, 2015-09-17 It has long been recognized that metal spin states play a central role in the reactivity of important biomolecules in industrial catalysis and in spin crossover compounds As the fields of inorganic chemistry and catalysis move towards the use of cheap non toxic first row transition metals it is essential to understand the important role of spin states in influencing molecular structure bonding and reactivity *Spin States in Biochemistry and Inorganic Chemistry* provides a complete picture on the importance of spin states for reactivity in biochemistry and inorganic chemistry presenting both theoretical and experimental perspectives The successes and pitfalls

of theoretical methods such as DFT ligand field theory and coupled cluster theory are discussed and these methods are applied in studies throughout the book Important spectroscopic techniques to determine spin states in transition metal complexes and proteins are explained and the use of NMR for the analysis of spin densities is described Topics covered include DFT and ab initio wavefunction approaches to spin states Experimental techniques for determining spin states Molecular discovery in spin crossover Multiple spin state scenarios in organometallic reactivity and gas phase reactions Transition metal complexes involving redox non innocent ligands Polynuclear iron sulfur clusters Molecular magnetism NMR analysis of spin densities This book is a valuable reference for researchers working in bioinorganic and inorganic chemistry computational chemistry organometallic chemistry catalysis spin crossover materials materials science biophysics and pharmaceutical chemistry

Molecular Electromagnetism: A Computational Chemistry Approach Stephan P. A. Sauer, 2011-08-25 This is a textbook on the theory and calculation of molecular electromagnetic and spectroscopic properties designed for a one semester course with lectures and exercise classes The idea of the book is to provide thorough background knowledge for the calculation of electromagnetic and spectroscopic properties of molecules with modern quantum chemical software packages The book covers the derivation of the molecular Hamiltonian in the presence of electromagnetic fields and of time independent and time dependent perturbation theory in the form of response theory It defines many molecular properties and spectral parameters and gives an introduction to modern computational chemistry methods

Electron Paramagnetic Resonance Marina Brustolon, Elio Giamello, 2009-02-25 This book offers a pragmatic guide to navigating through the complex maze of EPR ESR spectroscopy fundamentals techniques and applications Written for the scientist who is new to EPR spectroscopy the editors have prepared a volume that demystifies the basic fundamentals without weighting readers down with detailed physics and mathematics and then presents clear approaches in specific application areas The first part presents basic fundamentals and advantages of electron paramagnetic resonance spectroscopy The second part explores several application areas including chemistry biology medicine materials and geology A frequently asked questions section focuses on practical questions such as the size of sample etc It is an ideal hands on reference for chemists and researchers in the pharmaceutical and materials semiconductor industries who are looking for a basic introduction to EPR spectroscopy

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