Spin States In Biochemistry And Inorganic Chemist

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Departments of Labor, Health and Human Services, Education, and Related Agencies Appropriations for 1984 Morgan & Claypool Publishers

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.

Advances in Biological Solid-State NMR Royal Society of Chemistry

The idea that a long-lived form of spin order, namely singlet order, can be prepared from nuclear spin magnetisation first emerged in 2004. The unusual properties of singlet order–its long lifetime and the fact that it is NMR silent but interconvertible into other forms of NMR active order—make it a ‘smart tag’ that can be used to store information for a long time or through distant space points. It is

not unexpected then, that since its first appearance, this idea has caught the attention of research groups interested in exploiting this form of order in different fields of research spanning from biology to materials science and from hyperpolarisation to quantum computing. This first book on the subject gives a thorough description of the various aspects that affect the development of the topic and details the interdisciplinary applications. The book starts with a section dedicated to the basic theories of long-lived spin order and then proceeds with a description of the state-of-the-art experimental techniques developed to manipulate singlet order. It then concludes by covering the generalization of the concept of singlet order by introducing and discussing other forms of long-lived spin order.

NMR of Paramagnetic Molecules Springer Science & Business Media

The Chemistry and Biology of Nitroxyl (HNO) provides first-of-its-kind coverage of the intriguing biologically active molecule called nitroxyl, or azanone per IUPAC nomenclature, which has been traditionally elusive due to its intrinsically high reactivity. This useful resource provides the scientific basis to understand the chemistry, biology, and technical aspects needed to deal with HNO. Building on two decades of nitric oxide and nitroxyl research, the editors and authors have created an indispensable guide for investigators across a wide variety of areas of chemistry (inorganic, organic, organometallic, biochemistry, physical, and analytical); biology (molecular, cellular, physiological, and enzymology); pharmacy; and medicine. This book begins by exploring the unique molecule’s structure and reactivity, including important reactions with small molecules, thiols, porphyrins, and key proteins, before discussing chemical and biological sources of nitroxyl. Advanced chapters discuss methods for both trapping and detecting nitroxyl by spectroscopy, electrochemistry, and fluorescent inorganic cellular probing. Expanding on the compound’s foundational chemistry, this book then explores its molecular physiology to offer insight into its biological implications, pharmacological effects, and practical issues. Presents the first book on HNO (nitroxyl or azanone), an increasingly important molecule in biochemistry and pharmaceutical research Provides a valuable coverage of HNO’s chemical structure and significant reactions, including practical guidance on working with this highly reactive molecule Contains high quality content from recognized experts in both industry and academia

Quantum Chemistry and Dynamics of Excited States John Wiley & Sons

We present here the second issue devoted entirely to the spin-labeling technique as part of Biological Magnetic Resonance. Volume 14 commemorates a modifi- tion in our editorial policy with the retirement of my esteemed coeditor, Jacques Reuben. From thisjuncture into the future, each issue will focus on some special topic in magnetic resonance. Each volume will be organized in most cases by guest editors, for example forthcoming issues will address the following topics: in vivo magnetic resonance (P. Robitaille and L. J. Berliner, eds.) Modern techniques in proton NMR ofproteins (R. Krishna and L. J. Berliner, eds.) Instrumental techniques of EPR (C. Bender and L. J. Berliner, eds.) Thecurrent volume, Spin Labeling: The NextMillennium, presents an excellent collection of techniques and applications that evolved during the past decade since the last volume, volume 8 (1989). Someobvious omissions, such as multiquantum EPR and very high-frequency FT-ESR were unfortunately not possible for this volume. Perhaps they will appear in Spin Labeling: 2001. Lastly it is a pleasure to honor two scientists whose contributions were both pioneering and pivotal to the spin label technique: Professor Eduard G. Rozantsev (Moscow), whose synthetic feats in nitroxyl chemistry set the broad stage for a versatile catalog of labels; and Professor Harden M. McConnell, last year's Int- national ESR (EPR) Society Gold Medalist, who conceived and developed the spin label technique to address many biological problems (proteins, enzymes, m- branes, cells, immune response, etc.). Lawrence J.

Departments of Labor, Health and Human Services, Education, and related agencies appropriations for fiscal year 1984 Springer Science & Business Media

This is the first book covering all aspects of high pressure biochemistry and biophysics of proteins. Hydrostatic pressure is a powerful tool for study of biological systems. As a thermodynamic parameter, hydrostatic pressure has been known for a century to act on biological materials in a similar, but not identical, way to temperature. However, pressure was disregarded for a long time by biochemists mainly because the basic concepts (and the thermodynamics) focused on the chemical reactions involved and because general ideas on what pressure can add to the understanding of the behaviour of proteins were lacking. In recent decades, technological progress in the field of physics has shown, along with parameters such as temperature and solvent conditions, that pressure can be used for more refined thermodynamic and kinetic descriptions of biological processes and regulation of biological systems. The effects of pressure on proteins, nucleoproteins and membranes have recently been reviewed and several proceedings books have been published.

Transition Metals in Coordination Environments Springer Science & Business Media

During the past few decades we have witnessed an era of remarkable growth in the field of molecular biology. In 1950 very little was known of the chemical constitution of biological systems, the manner in which information was trans mitted from one organism to another, or the extent to which the chemical basis of life is unified. The picture today is dramatically different. We have an almost bewildering variety of information detailing many different aspects of life at the molecular level. These great advances have brought with them some breath-taking insights into the molecular mechanisms used by nature for rep licating, distributing and modifying biological information. We have learned a great deal about the chemical and physical nature of the macromolecular nucleic acids and proteins, and the manner in which carbohydrates, lipids and smaller molecules work together to provide the molecular setting of living sys tems. It might be said that these few decades have replaced a near vacuum of information with a very large surplus. It is in the context of this flood of information that this series of monographs on molecular biology has been organized. The idea is to bring together in one place, between the covers of one book, a concise assessment of the state of the subject in a well-defined field. This will enable the reader to get a sense of historical perspective-what is known about the field today-and a description of the frontiers of research where our knowledge is increasing steadily.

Nuclear Spin Relaxation in Liquids Springer Science & Business Media

Readership: Graduate students, researchers and industrialists in chemistry, physics and biology.

Spin Crossover in Transition Metal Compounds I Royal Society of Chemistry

Edited by Nobel Prize-winner Ilya Prigogine and renowned authority Stuart A. Rice, the Advances in Chemical Physics series provides a forum for critical, authoritative evaluations in every area of the discipline.

In a format that encourages the expression of individual points of view, experts in the field present comprehensive analyses of subjects of interest. This stand-alone, special topics volume, edited by Gert D. Billing of the University of Copenhagen and Michael Baer of the Soreq Nuclear Research Center in Yavne, Israel, reports recent advances on the role of degenerate states in chemistry. Volume 124 collects innovative papers on "Complex States of Simple Molecular Systems," "Electron Nuclear Dynamics," "Conical Intersections and the Spin-Orbit Interaction," and many more related topics. Advances in Chemical Physics remains the premier venue for presentations of new findings in its field.
Transition Metals in Biochemistry John Wiley & Sons
This book presents the versatile and pivotal role of electron spin interactions in nature. It provides the background, methodologies and tools for basic areas related to spin interactions, such as spin chemistry and biology, electron transfer, light energy conversion, photochemistry, radical reactions, magneto-chemistry and magneto-biology. The book also includes an overview of designing advanced magnetic materials, optical and spintronic devices and photo catalysts. This monograph will be of interest to scientists and graduate students working in the areas related to spin interactions physics, biophysics, chemistry and chemical engineering.
Cytochromes c Springer
This book focuses on the electronic properties of transition metals in coordination environments. These properties are responsible for the unique and intricate activity of transition metal sites in bio- and inorganic catalysis, but also pose challenges for both theoretical and experimental studies. Written by an international group of recognized experts, the book reviews recent advances in computational modeling and discusses their interplay using experiments. It covers a broad range of topics, including advanced computational methods for transition metal systems; spectroscopic, electrochemical and catalytic properties of transition metals in coordination environments; metalloenzymes and biomimetic compounds; and spin-related phenomena. As such, the book offers an invaluable resource for all researchers and postgraduate students interested in both fundamental and application-oriented research in the field of transition metal systems.
The Role of Degenerate States in Chemistry, Volume 124 Springer
Biological magnetic resonance (NMR and EPR) is a rapidly expanding area of research with much activity in most universities and research institutions. International conferences are held biennially with an increasing number of participants. With the introduction of sophisticated and continuously im proving instrumentation, biological magnetic resonance is approaching the state of a common physical method in biochemical, biomedical, and bio logical research. The lack of monograpbs on the subject had been con spicuous for a long time. This gap started to close only recently. However, because of the rapid expansion and intensive research, many texts are dated by the time of their appearance. Therefore we have undertaken the editing of a series that is intended to provide the practicing chemist, biochemist, or biologist with the advances and progress in selected contemporary topics. In seeking to make the series as authoritative as possible, we have invited authors who have not only made significant contributions but who are also currently active in their fields. We hope that their expertise as well as their first hand experience as reflected in the chapters of this volume will be of benefit to the reader, inter alia, in planning his own experiments and in critically evaluating the current literature.
Solid-State Spectroscopy John Wiley & Sons
With contributions by numerous experts
Departments of Labor, Health and Human Services, Education, and Related Agencies Appropriations for Fiscal Year 1984 Springer Science & Business Media
Nuclear Magnetic Resonance in Biochemistry: Principles and Applications focuses on the principles and applications of nuclear magnetic resonance (NMR) in biochemistry. Topics covered include experimental methods in NMR; the mechanisms of NMR relaxation; chemical and paramagnetic shifts; spin-spin splitting; the use of NMR in investigations of biopolymers and biomolecular interactions; and molecular dynamics in biological and biochemical systems. This text is comprised of eight chapters; the first of which gives an overview of NMR spectroscopy and its use in studies of biological systems. The next two chapters discuss the theoretical basis for NMR applications in biochemistry, with emphasis on Bloch equations, quantum mechanics, correlation function and correlation time, double resonance, and chemical exchange. The reader is then introduced to the basis for chemical shifts and spin-spin splitting, along with several examples of the use of these NMR parameters in studies of small molecule interactions and structure. The experimental apparatus and procedures employed in NMR studies, Fourier transform NMR, and NMR spectral parameters of small molecules interacting with macromolecules are also considered. The book highlights the information obtainable from the spectra of biopolymers, and then concludes with a chapter on NMR investigations of the state of motion of lipids in membranes and model membranes; water in macromolecular and cellular systems; and sodium ion in biological tissue. This book is intended primarily for chemists, biochemists, biophysicists, and molecular biologists, as well as graduate students.
Cooperativity Theory in Biochemistry Springer Science & Business Media
NMR of Paramagnetic Molecules: Principles and Applications is a compendium of papers that discusses the physical principles behind the technique of nuclear magnetic resonance, as well as, evaluates the scope and limitation of the applications of NMR in chemistry and biology. These papers emphasize the applications of the technique in chemistry and biochemistry where it widely used, particularlyon NMR experiments in the liquid state. Some papers describe the theoretical factors governing the resonance position and linewidth, and then also interpret magnetic resonance parameters in terms of electronic structure. Another paper investigates the gap between the mathematical complexities of earlier experiments and the operational aspects of chemical information from the spectra. Examples show studies in biochemical molecules and process in events where contact interactions are present either as a result of intrinsic molecular paramagnetism or are just induced through the addition of suitable paramagnetic probes. One paper presents the definitive and controversial results involving stereochemistry and deuterium NMR. This collection of papers will prove useful for nuclear physicists, researchers, and academicians in the field of nuclear physics.
Spin States in Biochemistry and Inorganic Chemistry Royal Society of Chemistry
Predicting molecular structure and energy and explaining the nature of bonding are central goals in quantum chemistry. With this book, the editors assert that the density functional (DF) method satisfies these goals and has come into its own as an advanced method of computational chemistry. The wealth of applications presented in the book, ranging from solid

state sys tems and polymers to organic and organo-metallic molecules, metallic clus ters, and biological complexes, prove that DF is becoming a widely used computational tool in chemistry. Progress in the methodology and its imple mentation documented by the contributions in this book demonstrate that DF calculations are both accurate and efficient. In fact, the results of DF calculations may pleasantly surprise many chem ists. Even the simplest approximation of DF, the local spin density method (LSD), yields molecular structures typical of ab initio correlated methods. The next level of theory, the nonlocal spin density method, predicts the energies of molecular processes within a few kcallmol or less. Like the Hartree-Fock (HF) and configuration interaction (CI) methods, the DF method is based only on fundamental physical constants. Therefore, it does not require semiempirical parameters and can be applied to any molecular system and to metallic phases. However, DF's greatest advantage is that it can be applied to much larger systems than those approachable by tradition al ab initio methods, especially when compared with correlated ab initio methods.

Quantum Biochemistry Springer Science & Business Media

Biomedical EPR – Part B focuses on applications of EPR techniques and instrumentation, with applications to dynamics. The book celebrates the 70th birthday of Prof. James S. Hyde, Medical College of Wisconsin, and his contributions to this field. Chapters are written to provide introductory material for new-comers to the field that lead into up-to-date reviews that provide perspective on the wide range of questions that can be addressed by EPR. Key Features: EPR Techniques including Saturation Recovery, ENDOR, ELDOR, and Saturation Transfer Instrumentation Innovations including Loop Gap Resonators, Rapid Mixing, and Time Locked Sub-Sampling Motion in Biological Membranes Applications to Structure Determination in Proteins Discussion of Trends in EPR Technology and Prognosis for the Future

Fundamental Laboratory Approaches for Biochemistry and Biotechnology John Wiley & Sons

The most complete and up-to-date survey of this important superfamily of enzymes, including the first ever coverage of the forms involved in steroid hormone biosynthesis. The components of the enzyme system, the reaction mechanisms involved, and the evolution and nomenclature are analyzed, as is the hepatic microsomal enzyme in a large number of species, illustrating the very wide implications for life processes.

Transition States of Biochemical Processes Springer Science & Business Media

Ninfa/Ballou/Benore is a solid biochemistry lab manual, dedicated to developing research skills in students, allowing them to learn techniques and develop the organizational approaches necessary to conduct laboratory research. Ninfa/Ballou/Benore focuses on basic biochemistry laboratory techniques with a few molecular biology exercises, a reflection of most courses which concentrate on traditional biochemistry experiments and techniques. The manual also includes an introduction to ethics in the laboratory, uncommon in similar manuals. Most importantly, perhaps, is the authors' three-pronged approach to encouraging students to think like a research scientist: first, the authors introduce the scientific method and the hypothesis as a framework for developing conclusive experiments; second, the manual's experiments are designed to become increasingly complex in order to teach more advanced techniques and analysis; finally, gradually, the students are required to devise their own protocols. In this way, students and instructors are able to break away from a "cookbook" approach and to think and investigate for themselves. Suitable for lower-level and upper-level courses; Ninfa spans these courses and can also be used for some first-year graduate work.

Electron Spin Interactions in Chemistry and Biology Springer

Nuclear magnetic resonance (NMR) is widely used across many fields because of the rich data it produces, and some of the most valuable data come from the study of nuclear spin relaxation in solution. While described to varying degrees in all major NMR books, spin relaxation is often perceived as a difficult, if not obscure, topic, and an accessible, cohesive treatment has been nearly impossible to find. Collecting relaxation theory, experimental techniques, and illustrative applications into a single volume, this book clarifies the nature of the phenomenon, shows how to study it, and explains why such studies are worthwhile. Coverage ranges from basic to rigorous theory and from simple to sophisticated experimental methods, and the level of detail is somewhat greater than most other NMR texts. Topics include cross-relaxation, multispin phenomena, relaxation studies of molecular dynamics and structure, and special topics such as relaxation in systems with quadrupolar nuclei and paramagnetic systems. Avoiding overly demanding mathematics, the authors explain relaxation in a manner that anyone with a basic familiarity with NMR can follow, regardless of their specialty. The focus is on illustrating and explaining the physical nature of the phenomena, rather than the intricate details. Nuclear Spin Relaxation in Liquids: Theory, Experiments, and Applications forms useful supplementary reading for graduate students and a valuable desk reference for NMR spectroscopists, whether in chemistry, physics, chemical physics, or biochemistry.

Cytochrome P450 World Scientific

EPR of Free Radicals in Solids: Trends in Methods and Applications, 2nd ed. presents a critical two volume review of the methods and applications of EPR (ESR) for the study of free radical processes in solids. Emphasis is on the progress made in the developments in EPR technology, in the application of sophisticated matrix isolation techniques and in the advancement in quantitative EPR that have occurred since the 1st edition was published. Improvements have been made also at theoretical level, with the development of methods based on first principles and their application to the calculation of magnetic properties as well as in spectral simulations. EPR of Free Radicals in Solids II focuses on the trends in applications of experimental and theoretical methods to extract structural and dynamical properties of radicals and spin probes in solid matrices by continuous wave (CW) and pulsed techniques in nine chapters written by experts in the field. It examines the studies involving radiation- and photo-induced inorganic and organic radicals in inert matrices, the high-spin molecules and metal-based molecular clusters as well as the radical pro-cesses in photosynthesis. Recent advancements in environmental applications in-cluding measurements by myon resonance of radicals on surfaces and by quantitative EPR in dosimetry are outlined and the applications of optical detection in material research with much increased sensitivity reviewed. The potential use of EPR in quantum computing is considered in a newly written chapter. This new edition is aimed to experimentalists and theoreticians in research involving free radicals, as well as for students of advanced courses in physical chemis-try, chemical physics, materials science, biophysics, biochemistry and related fields.