Electron Paramagnetic Resonance Of D Transition Metal Compounds

#electron paramagnetic resonance #d transition metal compounds #epr spectroscopy #transition metal complexes #paramagnetic materials

Explore the crucial role of Electron Paramagnetic Resonance (EPR) in unraveling the intricate electronic and magnetic properties of D transition metal compounds. This advanced spectroscopic technique offers unparalleled insights into oxidation states, spin dynamics, and ligand environments, making it indispensable for research in materials science and inorganic chemistry.

Electron Paramagnetic Resonance of d Transition Metal Compounds

Electron paramagnetic resonance (epr) spectroscopy is a sensitive and versatile method of studying paramagnets, which is finding increasing use in chemistry, biochemistry, earth and materials sciences. The technique is treated both qualitatively and quantitatively, with a progressive increase in sophistication in each succeeding chapter. Following a general introductory chapter, the first half of the book deals with single unpaired electron systems and considers both metal and ligand Zeeman, hyperfine and quadrupole interactions. The simulation of these spectra is discussed, followed by the relationship between spin-Hamiltonian parameters and models of the electronic structures of paramagnets. The second half of the book treats multiple unpaired electron systems using the same philosophy. An introduction to the epr properties of cluster compounds and of extended exchanging systems is also given. There is a chapter on linewidths and lineshapes, and an extensive appendix containing much additional information. A wide-ranging library of simulated and experimental spectra is given, as well as graphical data which should aid spectrum interpretation. Each chapter contains key references and there is a substantial subject and keyword index. This book is designed to teach epr spectroscopy to students without any previous knowledge of the technique. However, it will also be extremely useful to researchers dealing with paramagnetic d transition metals.

Electron Paramagnetic Resonance in Compounds of Transition Elements

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Electron Spin Resonance Studies of Early D-transition Metal Compounds with a D 1 -configuration

Reflecting the growing volume of published work in this field, researchers will find this book an invaluable source of information on current methods and applications.

Electron Paramagnetic Resonance in Compounds of Transition Elements

This introductory text on transition ion electron paramagnetic resonance is intended for beginning graduate students in physics and chemistry. The phenomenon studied is an important tool for the identification and characterization of transition and metal ions. The author presents a new perspective that unifies the main features of field-swept EPR of anisotropic systems, and accounts for the origin of asymmetric line shapes, linewidth anisotropy, and strain broadening. A large number of spectra are shown, since familiarity with the shape of typical spectra is essential for the proper employment of this technique. A wide range of examples are also provided, including transition ions in crystals, glasses, semiconductors, phase transitions, proteins and other biological systems. In addition to its value as a text, this work is suitable for scientists in a variety of disciplines, as well as for anyone whose work involves the use of transition ion EPR techniques.

Spin Crossover in Transition Metal Compounds II

There exists a large literature on the spectroscopic properties of copper(II) com- 9 pounds. This is due to the simplicity of the d electron configuration, the wide variety of stereochemistries that copper(II) compounds can adopt, and the f- xional geometric behavior that they sometimes exhibit [1]. The electronic and geometric properties of a molecule are inexorably linked and this is especially true with six-coordinate copper(II) compounds which are subject to a Jahn-T- ler effect.However,the spectral-structural correlations that are sometimes d- wn must often be viewed with caution as the information contained in a typical solution UV-Vis absorption spectrum of a copper(II) compound is limited. Meaningful spectral-structural correlations can be obtained in a related series of compounds where detailed spectroscopic data is available. In the fol- 4– lowing sections two such series are examined; the six-coordinate CuF and 6 2+ Cu(H O) ions doped as impurities in single crystal hosts.Using low tempera- 2 6 ture polarized optical spectroscopy and electron paramagnetic resonance, a very detailed picture can be drawn about the geometry of these ions in both their ground and excited electronic states. We then compare the spectrosco- cally determined structural data with that obtained from X-ray diffraction or EXAFS measurements.

Electron Paramagnetic Resonance in Compounds of Transition Elements

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.

Electron Paramagnetic Resonance

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Transition Ion Electron Paramagnetic Resonance

This series provides inorganic chemists and materials scientistswith a forum for critical, authoritative evaluations of advances inevery area of the discipline. Volume 58 continues to report recentadvances with a significant, up-to-date selection of contributionsby internationally-recognized researchers. The chapters of this volume are devoted to the followingtopics: • Tris(dithiolene) Chemistry: A Golden Jubilee • How to find an HNO needle in a (bio)-chemicalHaystack • Photoactive Metal Nitrosyl and Carbonyl Complexes Derivedfrom Designed Auxiliary Ligands: An Emerging Class ofPhotochemotherapeutics • Metal--Metal Bond-Containing Complexes as Catalysts forC--H Functionalization Iron Catalysis in Synthetic Chemistry • Reactive Transition Metal Nitride Complexes Suitable for inorganic chemists and materials scientists inacademia, government, and industries including pharmaceutical, finechemical, biotech, and agricultural.

Electron Paramagnetic Resonance of Transition Ions

Specialist Periodical Reports provide systematic and detailed review coverage of progress in the major areas of chemical research. Written by experts in their specialist fields the series creates a unique service for the active research chemist, supplying regular critical in-depth accounts of progress in particular areas of chemistry. For over 80 years the Royal Society of Chemistry and its predecessor, the Chemical Society, have been publishing reports charting developments in chemistry, which originally took the form of Annual Reports. However, by 1967 the whole spectrum of chemistry could no longer be contained within one volume and the series Specialist Periodical Reports was born. The Annual Reports themselves still existed but were divided into two, and subsequently three, volumes covering Inorganic, Organic and Physical Chemistry. For more general coverage of the highlights in chemistry they remain a 'must'. Since that time the SPR series has altered according to the fluctuating degree of activity in various fields of chemistry. Some titles have remained unchanged, while others have altered their emphasis along with their titles; some have been combined under a new name whereas others have had to be discontinued. The current list of Specialist Periodical Reports can be seen on the inside flap of this volume.

Transition Metal and Rare Earth Compounds

There exists a large literature on the spectroscopic properties of copper(II) com- 9 pounds. This is due to the simplicity of the d electron configuration, the wide variety of stereochemistries that copper(II) compounds can adopt, and the f- xional geometric behavior that they sometimes exhibit [1]. The electronic and geometric properties of a molecule are inexorably linked and this is especially true with six-coordinate copper(II) compounds which are subject to a Jahn-T- ler effect.However,the spectral-structural correlations that are sometimes d- wn must often be viewed with caution as the information contained in a typical solution UV-Vis absorption spectrum of a copper(II) compound is limited. Meaningful spectral-structural correlations can be obtained in a related series of compounds where detailed spectroscopic data is available. In the fol- 4– lowing sections two such series are examined; the six-coordinate CuF and 6 2+ Cu(H O) ions doped as impurities in single crystal hosts.Using low tempera- 2 6 ture polarized optical spectroscopy and electron paramagnetic resonance, a very detailed picture can be drawn about the geometry of these ions in both their ground and excited electronic

states. We then compare the spectrosco- cally determined structural data with that obtained from X-ray diffraction or EXAFS measurements.

High-field Electron Spin Resonance Study on Correlated Transition Metal Compounds and Metal-organic Compounds

Easy-to-follow guide helps you take full advantage of EPR spectroscopy's capabilities Electron Paramagnetic Resonance: A Practitioner's Toolkit serves as a practical guide that enables you to navigate through and make sense of the complex maze of electron paramagnetic resonance (EPR) spectroscopy fundamentals, techniques, and applications. The first half of this book is dedicated to explaining the core principles of EPR spectroscopy, using clear, easy-to-follow explanations and examples while avoiding complex physics and mathematics. The second half of the book focuses on applications, including problem-solving strategies for such fields as biology, medicine, material science, chemistry, physics, and radiation effects on matter. Carefully edited by two experienced EPR scientists, this book features a team of eighteen expert authors. Their contributions are based not only on a thorough examination and analysis of the primary literature, but also on their own firsthand experience in research and applications. As a result, the book is filled with practical advice, tips, and cautions addressing such issues as: Choosing the right experiment Selecting experimental parameters and sample size Avoiding setbacks and pitfalls Simulating the spectra With its straightforward explanations and clear examples, this book is just what researchers need to take full advantage of EPR spectroscopy's tremendous capabilities. It is particularly recommended for those interested in applications to chemistry, biology, medicine, and material science.

Calculation of NMR and EPR Parameters

Pulse EPR (electron paramagnetic resonance) is one of the newest and most widely used techniques for examining the structure, function and dynamics of biological systems and synthetic materials. Until now, however, there has been no single text dedicated to this growing area of research. This text addresses the need for a comprehensive overview of Pulse EPR. The book covers the basic theory of pulse EPR, as well as a description and critical evaluation of the existing and emerging methods needed for selecting and conducting the proper experiment and analyzing the results. This is an indispensable reference for all scientists who need a thorough grounding in this increasingly popular field of spectroscopy.

Transition Metal and Rare Earth Compounds

This book describes in mathematical terms the extraction of useful information from ESR spectra as applied to paramagnetic organic, inorganic and organometalic molecules. It lays a firm groundwork for understanding more sophisticated experiments, which the availability of newer commercial instruments has made possible. It takes the reader step by step through obtaining and interpretating ESR spectra of paramagnetic molecules. The mathematical basis of each observed phenomena are detailed and examples given. In particular there is a detailed discussion of 2nd order pertubation theory treatment of the Spin Hamiltonian for non-coincident G and A axes.

Electron Spin Resonance Line Widths of Transition Metal Ions and Complexes in Solution

This book provides an introduction to the underlying theory, fundamentals, and applications of EPR spectroscopy, as well as new developments in the area. Knowledge of the topics presented will allow the reader to interpret of a wide range of EPR spectra, as well as help them to apply EPR techniques to problem solving in a wide range of areas: organic, inorganic, biological, and analytical chemistry; chemical physics, geophysics, and minerology. Includes updated information on high frequency and multi-frequency EPR, pulsed microwave techniques and spectra analysis, dynamic effects, relaxation phenomena, computer-based spectra simulation, biomedical aspects of EPR, and more Equips readers with sufficient knowledge of EPR techniques to go on in their specialized area of interest Provides problem sets and concise bibliographies at the end of each chapter, plus several tutorial appendices on topics like mathematical operations, quantum mechanics of angular momentum, experimental considerations.

Progress in Inorganic Chemistry

The Proceedings in this volume are a refereed selection of presentations from The Third Asia-Pacific EPR/ESR Symposium (APES'01), held in Kobe, Japan from October 29 to November 1, 2001. Participants from 20 countries from Asia, Australia, Europe, North and South America presented 210 papers, of which 132 are included here. These Proceedings are also a blueprint for development of electron paramagnetic resonance (EPR) / electron spin resonance (ESR) in the Asia-Pacific region in the 21st century. The Symposium reflected a variety of research fields developed over half a century and focuses especially on the most recent developments, such as high-field and high-frequency EPR, which are envisaged to be further developed and applied to various fields in the 21st century. All sessions consisted of Plenary, Invited and Contributed presentations. The Plenary presentations aimed at summarizing the overall developments. Invited presentations, reviewing the most recent developments, and Contributed ones, dealing with original research recently carried out in the EPR/ESR area, were given in one of three parallel sessions. The unique research works presented cover various fields and reflect the existing diversity of applications of the EPR/ESR techniques.

Electron Spin Resonance

"Volume 31, devoted solely to the role of vanadium in life processes, offers a comprehensive and timely account of this fascinating field by 37 distinguished, international authorities. Highlights the properties of the various oxidation states of vanadium, their affinity for biogenic ligands, the effects of vanadium species on enzyme activity, the role of vanadium in nitrogenases and haloperoxidases, and more."

Electron Spin Resonance of Transition Metal Complexes

Inorganic and Bio-Inorganic Chemistry is the component of Encyclopedia of Chemical Sciences, Engineering and Technology Resources in the global Encyclopedia of Life Support Systems (EOLSS), which is an integrated compendium of twenty one Encyclopedias. The Theme on Inorganic and Bio-Inorganic Chemistry in the Encyclopedia of Chemical Sciences, Engineering and Technology Resources deals with the discipline which studies the chemistry of the elements of the period-ic table. It covers the following topics: From simple to complex compounds; Chemistry of metals; Inorganic synthesis; Radicals reactions with metal complexes in aqueous solutions; Magnetic and optical properties; Inorganometallic chemistry; High temperature materials and solid state chemistry; Inorganic biochemistry; Inorganic reaction mechanisms;Homogeneous and heterogeneous catalysis; Cluster and polynuclear compounds; Structure and bonding in inorganic chemistry; Synthesis and spectroscopy of transition metal complexes; Nanosystems;Computational inorganic chemistry; Energy and inorganic chemistry. These two volumes are aimed at the following five major target audiences: University and College students Educators, Professional practitioners, Research personnel and Policy analysts, managers, and decision makers and NGOs

Transition Metal and Rare Earth Compounds

This book covers the latest developments in metalloenzymes, including characterizing metal bridging in proteins and peptides, copper(II) complexes of marine peptides, high-spin Co(II) in model and metalloprotein systems to enzymes such as the molybdenum-containing enzymes, CW and pulse EPR of cytochrome P450 enzymes and the radical S-adenosylmethionine FeS family. In the previous two related volumes in the Biological Magnetic Resonance series, High-Resolution EPR: Applications to Metalloenzymes and Metals in Medicine and Metals in Biology:Applications of High-Resolution EPR to Metalloenzymes, topics covered included high-resolution EPR methods, iron proteins, nickel and copper enzymes, metals in medicine, iron–sulfur cluster-containing proteins, and molybdenum enzymes. In this volume, new developments in these areas are covered in detail and new areas that have emerged are also detailed. This is an ideal book for graduate students and researchers working in the fie lds of high-resolution EPR, metalloenzymes, and metals in biology.

Electron Paramagnetic Resonance

With its two-volume structure, this handbook and ready reference allows for comprehensive coverage of both characterization and applications, while uniform editing throughout ensures that the structure remains consistent. The result is an up-to-date review of metal oxides in catalysis. The first volume covers a range of techniques that are used to characterize oxides, with each chapter written by an expert in the field. Volume 2 goes on to cover the use of metal oxides in catalytic reactions. For all chemists and engineers working in the field of heterogeneous catalysis.

Principles of Pulse Electron Paramagnetic Resonance

Reflecting the growing volume of published work in this field, researchers will find this book an invaluable source of information on current methods and applications.

Studies of Nuclear Quadrupole Effects in Transition Metal Complexes by Electron Paramagnetic Resonance

Magnetic phenomena and materials are everywhere. Our understanding of magnetic behavior, once thought to be mature, has enjoyed new impetus from contributions ranging from molecular chemistry, materials chemistry and sciences to solid state physics. New phenomena are explored that open promising perspectives for commercial applications in future - carrying out chemical reactions in magnetic fields is just one of those. The spectrum spans molecule-based - organic, (bio)inorganic, and hybrid - compounds, metallic materials as well as their oxides forming thin films, nanoparticles, wires etc. Reflecting contemporary knowledge, this open series of volumes provides a much-needed comprehensive overview of this growing interdisciplinary field. Topical reviews written by foremost scientists explain the trends and latest advances in a clear and detailed way. By maintaining the balance between theory and experiment, the book provides a guide for both advanced students and specialists to this research area. It will help evaluate their own experimental observations and serve as a basis for the design of new magnetic materials. A unique reference work, indispensable for everyone concerned with the phenomena of magnetism!

Electron Spin Resonance

The expert authors of this monograph and professional reference include Dante Gatteschi, a pioneer of molecular magnetism. Based on the spin Hamiltonian approach, this unified treatment makes extensive use of irreducible tensor techniques to analyze systems in which two or more spins are magnetically coupled. 177 figures, 38 tables, and a new Introduction by Dr. Gatteschi. 1990 edition.

Electron Paramagnetic Resonance

Magnetochemistry is concerned with the study of magnetic properties in materials. It investigates the relationship between the magnetic properties of chemical compounds and their atomic and molecular structure. This rapidly growing field has a number of applications, and the measuring and interpreting of magnetic properties is often conducted by scientists who are not specialists in the field. Magnetochemistry requires complex mathematics and physics and so can be daunting for those who have not previously studied it in depth. Aimed at providing a single source of information on magnetochemistry, this book offers a comprehensive and contemporary review of the mathematical background and formula for predicting or fitting magnetic data, including a summary of the theory behind magnetochemistry to help understand the necessary calculations. Along with tables listing the key formula, there is also a model of the magnetic functions showing the effect of individual magnetic parameters. The clear structure and comprehensive coverage of all aspects of magnetochemistry will make this an essential book for advanced students and practitioners. Provides comprehensive overview of the mathematical background of magnetochemistry Uses clear and accessible language so scientists in a variety of fields can utilize the information Detailed explanations of equations and formula

Electron Paramagnetic Resonance of Ions Substituted Into Paramagnetic Transition Metal Ion Hosts

Specialist Periodical Reports provide systematic and detailed review coverage of progress in the major areas of chemical research. Written by experts in their specialist fields the series creates a unique service for the active research chemist, supplying regular critical in-depth accounts of progress in particular areas of chemistry. For over 80 years the Royal Society of Chemistry and its predecessor, the Chemical Society, have been publishing reports charting developments in chemistry, which originally took the form of Annual Reports. However, by 1967 the whole spectrum of chemistry could no longer be contained within one volume and the series Specialist Periodical Reports was born. The Annual Reports themselves still existed but were divided into two, and subsequently three, volumes covering Inorganic, Organic and Physical Chemistry. For more general coverage of the highlights in chemistry they remain a 'must'. Since that time the SPR series has altered according to the fluctuating degree of activity in various fields of chemistry. Some titles have remained unchanged, while others have altered their emphasis along with their titles; some have been combined under a new name whereas others

have had to be discontinued. The current list of Specialist Periodical Reports can be seen on the inside flap of this volume.

EPR in the 21st Century

Industrial and academic scientists face increasing challenges to find cost-effective and environmentally sound methods for converting natural resources into fuels, chemicals and energy. With over 7000 papers published in this field of catalysis each year, keeping up with the literature can be difficult. Catalysis Volume 27 presents critical and comprehensive reviews of the hottest literature published over the last twelve months. Covering major areas such as chemical transformations using two-dimensional hybrid nanocatalysts, conversion of biomass-derived syngas to fuels and catalytic oxidation of organic pollutants in aqueous solution using sulfate radicals, this book is a useful reference for anyone working in catalysis and an essential resource for any library.

Electron Paramagnetic Resonance of Exchange Coupled Systems

In keeping with goal and style of the Handbook in Modern Biophysics series, the proposed book will maintain a chapter structure that contains two parts: concepts and biological application. The book also integrates all the chapters into a smooth, continuous discourse. The first and second chapters establish the mathematical methods and theoretical framework underpinning the different topics in the rest if the book. Other chapters will use the theoretical framework as a basis to discuss optical and NMR approaches. Each chapter will contain innovative didactic elements that facilitate teaching, self-study, and research preparation (key points, summary, exercise, references).

Metal Ions in Biological Systems

Comprehensive, Up-to-Date Coverage of Spectroscopy Theory and its Applications to Biological Systems Although a multitude of books have been published about spectroscopy, most of them only occasionally refer to biological systems and the specific problems of biomolecular EPR (bioEPR). Biomolecular EPR Spectroscopy provides a practical introduction to bioEPR and demonstrates how this remarkable tool allows researchers to delve into the structural, functional, and analytical analysis of paramagnetic molecules found in the biochemistry of all species on the planet. A Must-Have Reference in an Intrinsically Multidisciplinary Field This authoritative reference seamlessly covers all important bioEPR applications, including low-spin and high-spin metalloproteins, spin traps and spin lables, interaction between active sites, and redox systems. It is loaded with practical tricks as well as do’s and don’ts that are based on the author’s 30 years of experience in the field. The book also comes with an unprecedented set of supporting software designed with simple graphical user interfaces that allow readers to tackle problems they will likely encounter when engaged in spectral analysis. Breaking with convention, the book broaches quantum mechanics from the perspective of biological relevance, emphasizing low-symmetry systems. This is a necessary approach since paramagnets in biomolecules typically have no symmetry. Where key topics related to quantum mechanics are addressed, the book offers a rigorous treatment in a style that is quick-to-grasp for the non expert. Biomolecular EPR Spectroscopy is a practical, all-inclusive reference sure to become the industry standard.

Inorganic and Bio-Inorganic Chemistry - Volume II

Determining the structure of molecules is a fundamental skill that all chemists must learn. Structural Methods in Molecular Inorganic Chemistry is designed to help readers interpret experimental data, understand the material published in modern journals of inorganic chemistry, and make decisions about what techniques will be the most useful in solving particular structural problems. Following a general introduction to the tools and concepts in structural chemistry, the following topics are covered in detail: • computational chemistry • nuclear magnetic resonance spectroscopy • electron paramagnetic resonance spectroscopy • Mössbauer spectroscopy • rotational spectra and rotational structure • vibrational spectroscopy • electronic characterization techniques • diffraction methods • mass spectrometry The final chapter presents a series of case histories, illustrating how chemists have applied a broad range of structural techniques to interpret and understand chemical systems. Throughout the textbook a strong connection is made between theoretical topics and the real world of practicing chemists. Each chapter concludes with problems and discussion questions, and a supporting website contains additional advanced material. Structural Methods in Molecular Inorganic Chemistry is an extensive update and sequel to the successful textbook Structural Methods in Inorganic Chemistry

by Ebsworth, Rankin and Cradock. It is essential reading for all advanced students of chemistry, and a handy reference source for the professional chemist.

Future Directions in Metalloprotein and Metalloenzyme Research

Metal Oxide Catalysis, 2 Volume Set