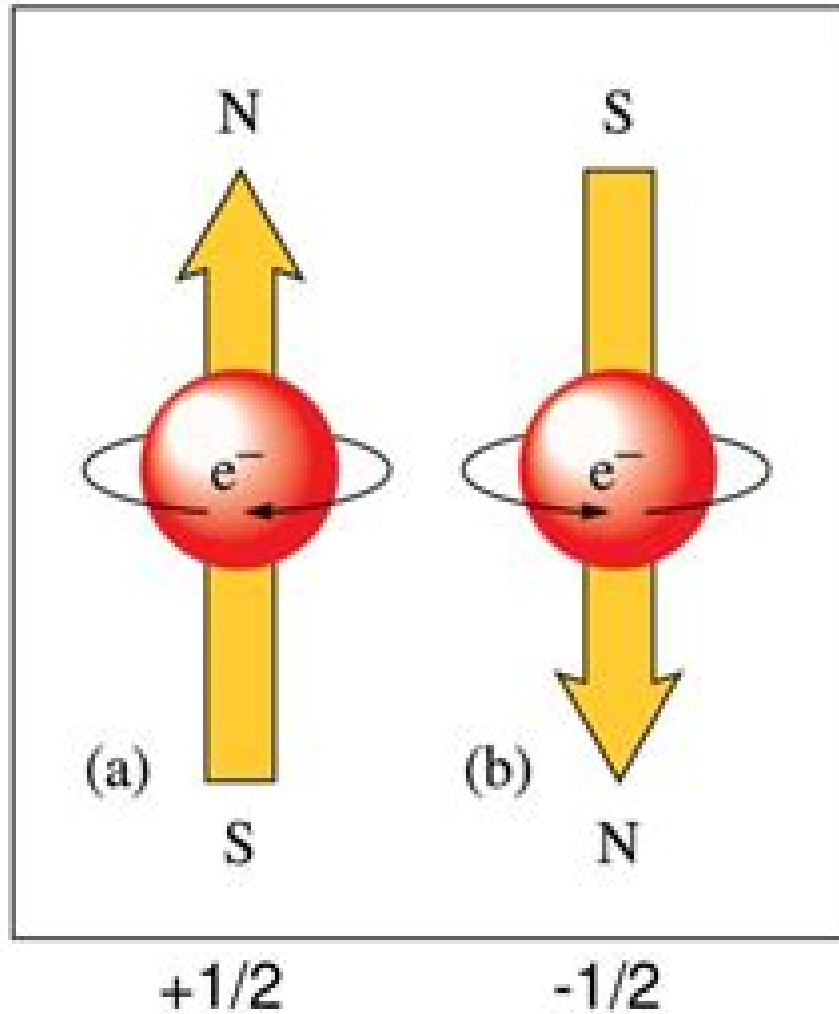


# Electron Spin



- **Opposite spins produce opposite magnetic fields.**

# Spins In Chemistry Current Chemical Concepts

**J.M. García de la Vega, J. San Fabián**



## **Spins In Chemistry Current Chemical Concepts:**

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Transfer Reactions of Complex Ions in Solution covers the significant development of some important area of electron transfer reactions of complex ions This four chapter book emerged from a series of lectures at the Polytechnic Institute of Brooklyn in November and December 1967 Chapter I presents research studies in cation hydration This chapter describes principal methods for composition determination of the first coordination spheres of the aquo ions Chapter II examines the distinction between reactions in which electron transfer takes place from one primary bond system to another Chapter III discusses some aspects of ligand effects in electron transfer reactions This chapter demonstrates that differences in the behavior of systems can be expected at least in the extremes of mechanisms Chapter IV deals with the history principles and applications of the induced electron transfer effect This book is of great value to electrochemists students and researchers

**Current Catalog** , 1965 First multi year cumulation covers six years 1965 70      The Publishers' Trade List Annual , 1978

*New Frontiers in Nanochemistry: Concepts, Theories, and Trends* Mihai Putz, 2020-05-10 New Frontiers in Nanochemistry Concepts Theories and Trends Volume 1 Structural Nanochemistry is the first volume of the new three volume set that explains and explores the important concepts from various areas within the nanosciences This first volume focuses on structural nanochemistry and encompasses the general fundamental aspects of nanochemistry while simultaneously incorporating crucial material from other fields in particular mathematic and natural sciences with specific attention to multidisciplinary chemistry Under the broad expertise of the editor the volume contains 50 concise yet comprehensive entries from world renowned scholars alphabetically organizing a multitude of essential basic and advanced concepts ranging from algebraic chemistry to new energy technology from the bondonic theory of chemistry to spintronics and from fractal dimension and kinetics to quantum dots and tight binding and much more The entries contain definitions short characterizations uses and usefulness limitations references and more      New Frontiers in Nanochemistry: Concepts, Theories, and Trends, 3-Volume Set Mihai V. Putz, 2022-05-29 New Frontiers in Nanochemistry Concepts Theories and Trends 3 Volume Set explains and explores the important fundamental and advanced modern concepts from various areas of nanochemistry and more broadly the nanosciences This innovative and one of a kind set consists of three volumes that focus on structural nanochemistry topological nanochemistry and sustainable nanochemistry respectively collectively forming an explicative handbook in nanochemistry The compilation provides a rich resource that is both thorough and accessible encompassing the core concepts of multiple areas of nanochemistry It also explores the content through a trans disciplinary lens integrating the basic and advanced modern concepts in nanochemistry with various examples applications issues tools

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**Spin Chemical Physics of Graphene** Elena Sheka, 2017-11-23 Graphene's nickname miracle material normally means the material superior properties. However, all these characteristics are only the outward manifestation of the wonderful nature of graphene. The real miracle of graphene is that the species is a union of two entities: a physical and a chemical one, each of which is unique in its own way. The book concerns a very close interrelationship between graphene physics and chemistry as expressed via typical spin effects of a chemical physics origin. Based on quantum chemical computations, the book is nevertheless addressed to the reflection of physical reality and it is aimed at an understanding of what constitutes graphene as an object of material science: graphene on the one hand and as a working material, high-tech graphene, for a variety of attractive applications, largely discussed and debated in the press on the other. The book is written by a user of quantum chemistry sufficiently experienced in material science and the chemical physics of graphene is presented as the user view based on results of extended computational experiments in tight connection with their relevance to physical and chemical realities. The experiments have been carried out at the same theoretical platform which allows considering different sides of the graphene life at the same level in light of its chemical peculiarity.

*Exploring Chemical Concepts Through Theory and Computation* Shubin Liu, 2024-12-23 Deep theoretical resource on the essence of chemistry explaining a variety of important concepts including redox states and bond types. *Exploring Chemical Concepts Through Theory and Computation* provides a comprehensive account of how the three widely used theoretical frameworks of valence bond theory, molecular orbital theory, and density functional theory, along with a variety of important chemical concepts, can between them describe and efficiently and reliably predict key chemical parameters and phenomena. By comparing the three main theoretical frameworks, readers will become competent in choosing the right modeling approach for their task. The authors go beyond a simple comparison of existing algorithms to show how data-driven theories can explain why chemical compounds behave the way they do, thus promoting a deeper understanding of the essence of chemistry. The text is contributed to by top theoretical and computational chemists who have turned computational chemistry into today's data-driven and application-oriented science. *Exploring Chemical Concepts Through Theory and Computation* discusses topics including orbital-based approaches, density-based approaches, chemical bonding, partial charges, atoms in molecules, oxidation states, aromaticity and antiaromaticity, and acidity and basicity, electronegativity, hardness, softness, HSAB, sigma-hole interactions, charge transport and energy transfer, and homogeneous and heterogeneous catalysis, electrophilicity, nucleophilicity, cooperativity, frustration, homochirality, and energy decomposition. Chemical concepts in solids, excited states, spectroscopy, and machine learning, and catalysis and machine learning, as well as key connections between related concepts. Aimed at both novice and experienced computational, theoretical, and physical chemists, *Exploring Chemical Concepts Through Theory and Computation* is an essential reference to gain a deeper, more advanced, holistic understanding of the

field of chemistry as a whole      **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      **Publishers' Trade List Annual, 1980** Bobbs-Merrill Educational Co, 1980      **Chemistry: The Central Science** Theodore L. Brown, H. Eugene LeMay Jr., Bruce E. Bursten, Catherine Murphy, Patrick Woodward, Steven Langford, Dalius Sagatys, Adrian George, 2013-10-04 If you think you know the Brown LeMay Bursten Chemistry text think again In response to market request we have created the third Australian edition of the US bestseller Chemistry The Central Science An extensive revision has taken this text to new heights Triple checked for scientific accuracy and consistency this edition is a more seamless and cohesive product yet retains the clarity innovative pedagogy functional problem solving and visuals of the previous version All artwork and images are now consistent in quality across the entire text And with a more traditional and logical organisation of the Organic Chemistry content this comprehensive text is the source of all the information and practice problems students are likely to need for conceptual understanding development of problem solving skills reference and test preparation      **The Chemistry of Alkanes and Cycloalkanes** Saul Patai, Zvi Rappoport, 1992-05-25 Multinational contributors provide extensive coverage regarding the synthesis and properties of this important functional group Structural chemistry NMR and mass spectrometry analytical factors such as thermochemistry reactivity namely electrophilic acidity basicity and rearrangements natural occurrence and biochemistry are among the subjects discussed      *Advances in Photochemistry, Volume 23* Douglas C. Neckers, David H. Volman, Günther von Büнау, 2009-09-24 Setting the pace for progress and innovation ADVANCES IN PHOTOCHEMISTRY More than a simple survey of the current literature Advances in Photochemistry offers critical evaluations written by internationally recognized experts These pioneering scientists offer unique and varied points of view of the existing data Their articles are challenging as well as provocative and are intended to stimulate discussion promote further research and encourage new developments

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**The Pauli Exclusion Principle** Ilya G. Kaplan, 2017-01-17 This is the first scientific book devoted to the Pauli exclusion principle which is a fundamental principle of quantum mechanics and is permanently applied in chemistry physics and molecular biology However while the principle has been studied for more than 90 years rigorous theoretical foundations still have not been established and many unsolved problems remain Following a historical survey in Chapter 1 the book discusses the still unresolved questions around this fundamental principle For instance why according to the Pauli exclusion principle are only symmetric and antisymmetric permutation symmetries for identical particles realized while the Schrödinger equation is satisfied by functions with any permutation symmetry Chapter 3 covers possible answers to this question The construction of function with a given permutation symmetry is described in the previous Chapter 2 while Chapter 4 presents effective and elegant methods for finding the Pauli allowed states in atomic molecular and nuclear spectroscopy Chapter 5 discusses parastatistics and fractional statistics demonstrating that the quasiparticles in a periodical lattice including excitons and magnons are obeying modified parafermi statistics With detailed appendices The Pauli Exclusion Principle Origin Verifications and Applications is intended as a self sufficient guide for graduate students and academic researchers in the fields of chemistry physics molecular biology and applied mathematics It will be a valuable resource for any reader interested in the foundations of quantum mechanics and its applications including areas such as atomic and molecular spectroscopy spintronics theoretical chemistry and applied fields of quantum information

High Resolution NMR Spectroscopy J.M. García de la Vega, J. San Fabián, 2013-06-08 Natural bond orbital and natural J coupling methods are used for the analysis of the Fermi contact contributions to spin spin coupling constant SSCC In this way the SSCCs are partitioned into three contributions Lewis delocalization and repolarization This partition is applied to the study of some chemical systems to explain the main electron delocalization effects on SSCCs

**Subject Guide to Books in Print**, 1984

Advances in Quantum Chemistry, 1994-05-11 Advances in Quantum Chemistry

**Handbook of Research on Science Education, Volume II** Norman G. Lederman, Sandra K. Abell, 2014-07-11 Building on the foundation set in Volume I a landmark synthesis of research in the field Volume II is a comprehensive state of the art new volume highlighting new and emerging research perspectives The contributors all experts in their research areas represent the international and gender diversity in the science education research community The volume is organized around six themes theory and methods of science education research science learning culture gender and society and science learning science teaching curriculum

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