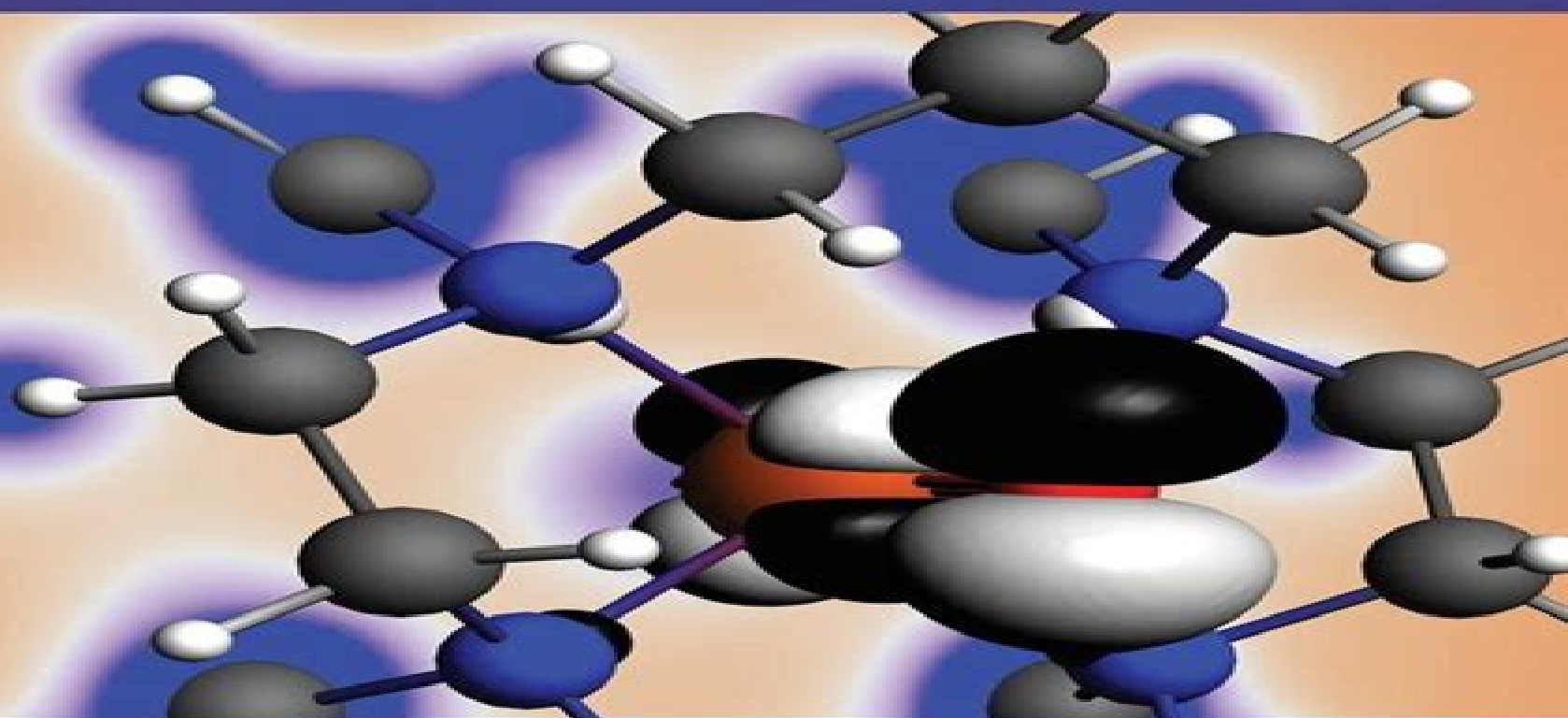


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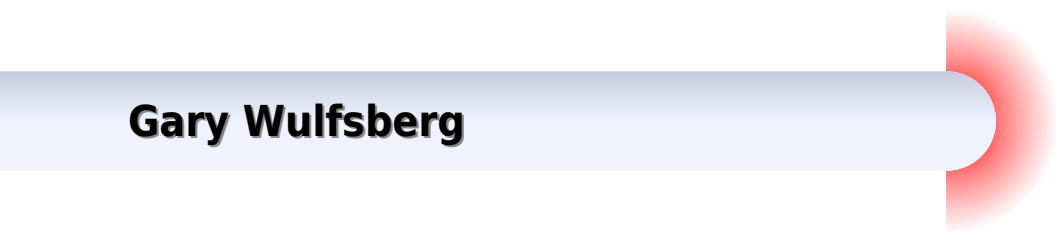
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Nice Book Spin States Biochemistry Inorganic Chemistry

Gary Wulfsberg



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Spin States in Biochemistry and Inorganic Chemistry Marcel Swart, Miquel Costas, 2015-12-14 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 science, biophysics and pharmaceutical chemistry.

Transition Metals in Coordination Environments Ewa Broclawik, Tomasz Borowski, Mariusz Radoń, 2019-03-16 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.

Practical Approaches to Biological Inorganic Chemistry Robert R. Crichton, Ricardo O. Louro, 2019-09-10 *Practical Approaches to Biological Inorganic Chemistry* Second Edition reviews the use of spectroscopic and related analytical techniques to investigate the complex structures and mechanisms of biological inorganic systems that contain metals. Each chapter presents an overview of the technique, including relevant theory, a clear explanation of what it is, how it works and how the technique is actually used to evaluate biological structures. New chapters cover Raman Spectroscopy and Molecular Magnetochemistry, but all chapters have been updated to reflect the latest developments in discussed techniques.

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