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of the Tetrapyrroles; 2.3.1 Introduction
 2.3.2 Spin States
 2.3.3 Tetrapyrroles Prefer Their Native Ions; 2.3.4
 Cavity Size and Flexibility of the Tetrapyrroles; 2.3.5 Cytochrome-like
 Electron Transfer; 2.3.6 Stability of a Metal-Carbon Bond; 2.3.7
 Metallation Reaction; 2.4 Tuning of Tetrapyrrole Structure and Function
 by Axial Ligands; 2.4.1 Introduction; 2.4.2 Importance of the Lower
 Axial Ligand for B(12) Chemistry; 2.4.3 Lower Axial Ligand in Cofactor
 F430; 2.4.4 Importance of Axial Ligands for the Globins; 2.4.5 Role of
 Axial Ligands for the Cytochromes; 2.4.6 Role of the Axial Ligand in
 Heme Enzymes
 2.4.7 Tuning the His Ligand by Hydrogen Bonds in Heme Proteins
 2.4.8 Axial Ligand in Chlorophylls; 2.5 Concluding Remarks; References; 3
 Modeling of Mechanisms for Metalloenzymes where Protons and
 Electrons Enter or Leave; 3.1 Introduction; 3.2 Energy Diagrams; 3.2.1
 Photosystem II; 3.2.2 Cytochrome c Oxidase; 3.2.3 Nitric Oxide
 Reduction; 3.2.4 NiFe-hydrogenase; 3.2.5 Molybdenum CO
 Dehydrogenase; 3.3 Conclusions; References; 4 Principles of Dinitrogen
 Hydrogenation: Computational Insights; 4.1 Introduction
 4.2 Reaction Mechanism of the Coordinated Dinitrogen Molecule in Di-
 zirconocene-N(2) Complexes with a Hydrogen Molecule
 4.2.1 Mechanism of the Reaction (3); 4.2.2 Mechanisms of the Reactions (4)
 and (5); 4.3 Factors Controlling the N(2) Coordination Modes in the Di-
 zirconocene-N(2) Complexes; 4.4 Why the $[(\eta^5\text{-C}_5\text{Me}_5)_2\text{Ti}(\text{N}_2)]$
 $[(\eta^5\text{-C}_5\text{Me}_5)_2\text{Zr}(\text{N}_2)]$ Complex Cannot Add a H(2) Molecule to the
 Side-on Coordinated N(2), while its Zr- and Hf-analogs Can
 4.4.1 Relative Stability of the Lowest Singlet (S) and Triplet (T) Electronic
 States of the Complexes $[(\eta^5\text{-C}_5\text{Me}_5)_2\text{M}(\text{N}_2)]$ (for M = Ti, Zr, and Hf, and n = 0 and 4)

Sommario/riassunto

Here, the world's most active and productive computational scientists from academia and industry present established, effective and powerful tools for understanding catalysts. With its broad scope -- nitrogen fixation, polymerization, C-H bond activation, oxidations, biocatalysis and much more -- this book represents an extensive knowledge base for designing efficient catalysts, allowing readers to improve the performance of their own catalysts.