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Hydrogenases - Proton and Dihydrogen Activation; Chapter 3 [NiFe] Hydrogenases; 3.1 Introduction; 3.2 Introduction to [NiFe] Hydrogenases; 3.3 Nickel Thiolate Complexes as Analogs of [NiFe] Hydrogenase; 3.4 [NiFe] Hydrogenase Model Complexes; 3.4.1 Amine [N₂Ni(-S₂)Fe] Complexes; 3.4.2 Phosphine [P₂Ni(-S₂)Fe] Complexes; 3.4.3 Thiolate [S_xNi(-S_y)Fe] Complexes; 3.4.4 Polymetallic [Ni(-S)_zFe_y] Complexes; 3.5 Analogs of [NiFe] Hydrogenase Incorporating Proton Relays; 3.5.1 Nickel Complexes Incorporating Protonation Sites 3.5.2 [NiFe] Complexes Incorporating Protonation Sites 3.6 Perspectives and Future Challenges; Acknowledgments; References; Chapter 4 [FeFe] Hydrogenase Models: an Overview; 4.1 Introduction; 4.2 Synthetic Strategies toward [FeFe] Hydrogenase Model Complexes; 4.3 Properties of Model Complexes; 4.3.1 Biomimetic Models of the "Rotated State"; 4.3.2 Electron Transfer in [FeFe] Hydrogenase Models; 4.3.3 Protonation Chemistry of [FeFe] Hydrogenase Models; 4.3.3.1 Hydride Formation; 4.3.3.2 Ligand Protonation and Proton Relays; 4.3.4 Water-Soluble Hydrogenase Mimics; 4.4 Conclusion; References Chapter 5 The Third Hydrogenase 5.1 Introduction; 5.2 Initial Studies of Hmd; 5.3 Discovery that Hmd Contains a Bound Cofactor; 5.4 Discovery that Hmd is a Metalloenzyme; 5.5 Crystal Structure Studies of [Fe] Hydrogenase; 5.6 Mechanistic Models of [Fe] Hydrogenase; 5.6.1 Studies Before the Most Recent Assignment of the FeGP Cofactor; 5.6.2 Studies After the Most Recent Assignment of the FeGP Cofactor; 5.6.3 Synthesized Model Complexes of the FeGP Cofactor; References; Chapter 6 DFT Investigation of Models Related to the Active Site of Hydrogenases; 6.1 Introduction 6.2 QM Studies of Hydrogenases

Sommario/riassunto

This book provides an overview of bioinspired metal-sulfur catalysis by covering structures, activities and model complexes of enzymes exhibiting metal sulphur moieties in their active center.
