

Correlation of Structures and Reactivity of Bispidine Coordination Compounds

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Bispidine-type ligands are relatively easy to synthesize, and a large number of tetra-, penta- and hexadentate ligands, including chiral and dinucleating ligands with a variety of donor groups are available (shown in the Figure is a tetradentate ligand and the simplified structure of the corresponding metal complex with two monodentate co-ligands).



The very rigid ligand structures and the elasticity of the coordination sphere, as well as the enforced octahedral geometry with two electronically and structurally distinct sites for substrate coordination lead interesting molecular properties: μ -peroxodicycopper(II) complexes with dinucleating bispidine ligands are among the most stable examples known today, four coordination modes of catechol to copper(II) have been observed, structurally characterized and found to exhibit catechol oxidase activity, “Jahn-Teller isomers” have been observed and analyzed in detail, the iron(II)/H₂O₂ system is an efficient oxidation catalyst and various mechanistic pathways have been found and analyzed in detail. These and other properties are interpreted on the basis of X-ray data, DFT, MM and ligand field calculations, and the molecular properties are found to strongly correlate with specific structural parameters.

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