Copper(II) complexes containing pyridine-based and phenolate-based systems: Synthesis, characterization, DFT study, biomimetic catalytic activity of catechol oxidase and phenoxazinone synthase

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Abstract:

A template Schiff condensation of 2,6-pyridine dicarbaldehyde or 2,6-diformyl-4-bromophenol and 1,3-diamino-2-hydroxy propane or 3,4-diaminotoluene in the presence of copper(II) salts (CuX2) (X = Cl, Br, CH3COO, or ClO4) affords different types of copper(II) complexes. Depending on the employed molar ratio of the dicarbonyl compounds and diamines, different types of copper(II) complexes formed during the template condensation reaction. Structural formulation of the complexes was confirmed by elemental analysis (C, H, N, and M), physical measurements such as thermal analysis (TAG & DTG), molar conductivity, and magnetic moments in addition to spectral studies (UV-Vis, IR, and ESR). Homobinuclear in a four-coordinate square planar and five-coordinate square pyramidal and trigonal bipyramidal in monomeric structures are proposed. A mononuclear hexa-coordinate in an octahedral geometry is suggested as well. Oxidase biomimetic catalytic activity of these newly synthesized copper(II) complexes was examined toward the aerobic oxidation of 4-tert-butylcatechol (4-TBCH2) and oaminophenol under catalytic conditions. Both catalytic and kinetic investigations demonstrate promising oxidase catalytic activity and based on the kinetic results, probable mechanistic catalytic implications are discussed. Geometrical structures of representative copper(II) complexes were determined by optimizing their bond lengths, bond angles, dihedral angles, and the structural index (τ).

Keywords:

biomimetic catalytic activity, catechol oxidase, copper(II) complexes, Phenoxazinone synthase, pyridine-based and phenolate-based ligands

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