Title:	Copper(II) complexes with a benzimidazole functionalized Schiff base: Synthesis, crystal structures, and role of ancillary ions in phenoxazinone synthase activity
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Keywords:	Synthesis crystal structures
Issue Date:	2021
Publisher:	Wiley
Citation:	Applied Organometallic Chemistry, 35(6).
Abstract:	This research study reports the synthesis, structural characterization and phenoxazinone synthase-like activity of two structurally similar copper(II) complexes developed with a benzimidazole functionalized Schiff base (L). The ligand, L, was designed and synthesized in high yield by the reaction of p-methoxy benzaldehyde with o-phenylenediamine. The reaction of L with CuCl2 and Cu(NO3)2 leads to the formation of two isostructural complexes, [Cu(L)2Cl2]2 (1) and [Cu(L)2(NO3)2]2 (2). Single crystal X-ray structural study reveals that both the Cu(II) centre in 1 and 2 adopts a square planar geometry. An attempt has also been made to understand the role of coordinated co-ligands on the catalytic oxidation of 2-aminophenol (2-AP) to 2-amino-3H-phenoxazine-3-one (2-APX) in methanol. The presence of coordinated nitrate to Cu(II) ions imparts a more labile character to complex 2, and the catalytic efficiency (kcat/KM) for complex 2 (1.50 × 107) was determined almost double compared with that of complex 1 (8.78 × 106). Electro-chemical and electrospray ionization mass spectrometry studies of 1 and 2 with 2-AP suggests that the square planar geometries of the Cu(II) centres remain the driving force to develop enzyme-substrate adducts and excellent catalytic performance of the complexes. Electrochemical and EPR spectral analysis of the reaction mixture confirm the presence of active 2-AP−/2-AP•− redox species in the course of catalytic oxidation and suggest the radical driven oxidative coupling of 2-AP in an aerobic environment. Temperature-dependent kinetic measurements were carried out to evaluate the activation parameters (Ea, ΔH‡, ΔS‡), which favours the higher rate of catalytic oxidation of 2-AP for complex 2 than complex 1.
Description:	Only IISER Mohali authors are available in the record.
URI:	https://onlinelibrary.wiley.com/doi/10.1002/aoc.6211 (https://onlinelibrary.wiley.com/doi/10.1002/aoc.6211) http://hdl.handle.net/123456789/5026 (http://hdl.handle.net/123456789/5026)
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