

Synthesis, spectroscopic depiction and phenoxazinone synthase activity by a cobalt(II) complex

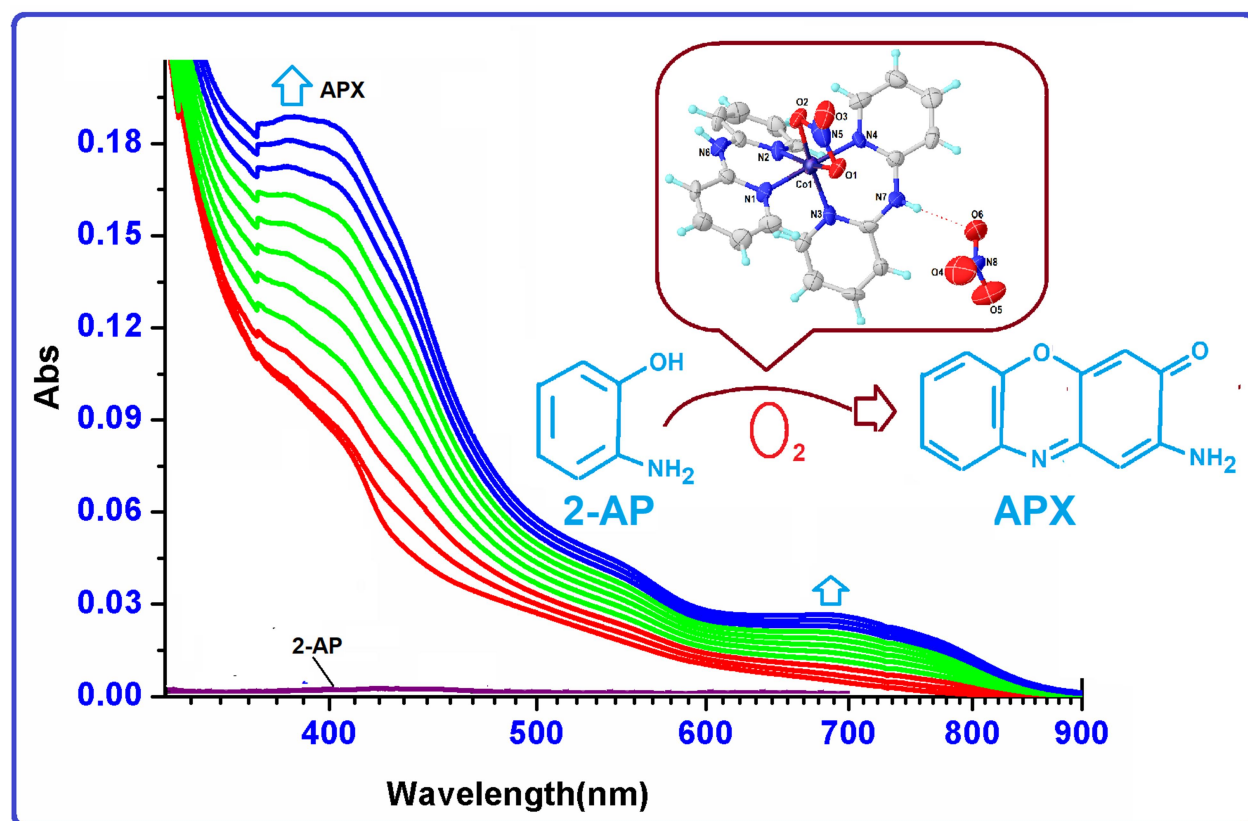
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Abstract:

Synthesis and structural characterization of a cobalt(II) complex, [Co(2,2'-dpa)₂(NO₃)₂]_nNO₃ (1) [2,2'-dpa = 2,2'-dipyridylamine] has been reported. Single crystal X-ray diffraction study reveals that 1 crystallizes in monoclinic system with *P*2₁/*n* space group. Investigation on supramolecular investigation reveals that counter anionic nitrate ion plays a crucial role in the construction of long range 3D crystalline structure. Room temperature magnetic susceptibility measurement

predicts the high spin nature of the cobalt(II) compound. The cobalt(II) complex has been evaluated to mimics the functional sites of phenoxazinone synthase enzyme in acetonitrile medium. The cobalt(II) complex significantly able to promote the oxidative coupling of 2-aminophenol (2-AP) to 2-aminophenoxazin-3-one under aerobic condition with significant turn over number, $k_{\text{cat}} = 1.46 \times 10^4 \text{ h}^{-1}$. ESI-MS of the reaction mixture recommends that the course of catalysis proceeds through substrate-enzyme adduct formation. Finally, detailed quantum chemical calculations have firmly supported the experimental observations.

Keywords: Bio-inorganic chemistry, Cobalt(II), Density functional theory, Phenoxazinone Synthase activity, X-ray structure