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Title:	Schiff base triggering synthesis of copper(II) complex and its catalytic fate towards mimics of phenoxazinone synthase activity
Authors:	Joshi, Mayank (/jspui/browse?type=author&value=Joshi%2C+Mayank) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Copper(II) Schiff base X-ray structure Phenoxazinone synthase activity DFT study
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Abstract:	This research article reports the synthesis, structural characterization and phenoxazinone synthase activity of a new phenoxido-bridged dicopper(II)-Schiff base complex, [Cu ₂ (L) ₃ ClO ₄ (1), [HL = (Z)-2-methoxy-6-((2-methoxyphenyl)imino) methyl]phenol]. X-ray structure of the Cu(II) complex reveals that each of the two Cu(II) centres in 1 adopts different coordination geometries (distorted octahedral and distorted square planar) and phenoxido bridges couple two Cu(II) centres to form a dinuclear copper complex with Cu...Cu distance 3.182 Å. The dicopper(II) complex catalyzes the aerobic oxidation of 2-aminophenol (2-AP) to aminophenoxazinone species in acetonitrile with good turnover number, 78.14 h ⁻¹ . Electro-chemical and electrospray ionization mass spectrometry analysis of 1 in presence of 2-AP ensure the involvement and key role of the copper(II) centres in formation of enzyme-substrate adduct. Subsequently, electron paramagnetic resonance study confirms the generation of radical species in the course of catalysis. Finally, density functional theoretical calculations well reproduce the experimental geometrical parameters and spectroscopic behaviours of 1 and decisively argue in favour of the proposed catalytic pathways.
Description:	Only IISERM authors are available in the record.
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