Title:	Ligand directed synthesis of a unprecedented tetragonalbipyramidal copper (II) complex and its antibacterial activity and catalytic role in oxidative dimerisation of 2-aminophenol
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Abstract:	In pursuit of the significant contribution of copper ion in different biological processes, this research work describes the synthesis, X-ray structure, Hirshfeld surface analysis, oxidative dimerization of 2-aminophenol and antibacterial activity of a newly designed copper (II)-Schiff base complex, [Cu(L)2] (1), [Schiff base (HL) = 2-(2-methoxybenzylideneamino)phenol]. X-ray structural analysis of 1 reveals that the Cu (II) complex crystallizes in a cubic crystal system with Ia-3d space group. The Cu (II) centre adopts an unprecedented tetragonal bipyramidal geometry in its crystalline phase. The Schiff base behaves as a tridentate chelator and forms an innermetallic chelate of first order with Cu (II) ion. The copper (II) complex has been tested in the bio-mimics of phenaxozinone synthase activity in acetonitrile and exhibits good catalytic activity as evident from high turnover number, 536.4 h−1. Electrochemical analysis exhibits the appearance of two additional peaks at −0.15 and 0.46 V for Cu (II) complex in presence of 2-AP and suggests the development of AP−/AP•− and AP•−/IQ redox couples in solution, respectively. The presence of iminobenzosemiquinone radical at g = 2.057 in the reaction mixture was confirmed by electron paramagnetic resonance and may be considered the driving force for the oxidative dimerisation of 2-AP. The existence of a peak at m/z 624.81 for Cu (II) complex in presence of 2-AP in electrospray ionization mass spectrum ensures that the catalytic oxidation proceeds through enzyme-substrate adduct formation. The copper (II) complex exhibits potential antibacterial properties against few pathogenic bacterial species like Staphylococcus aureus, Enterococcus and Klebsiella pneumonia and scanning electron microscope studies consolidates that destruction of bacterial cell membrane accounts on the development of antibacterial activity.
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