Title:	Ligand-Centered Radical Activity by a Zinc-Schiff-Base Complex towards Catechol Oxidation
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Abstract:	In this work, we present the synthesis and structural characterization of a new Zn(II)-Schiff base complex, [Zn(L)(H2O)] (1), [L=N,N′-bis(3-methoxysalicylidene)-1,3-diamino-2-propanol]. Single crystal X-ray structural analysis reveals that 1 crystallizes in monoclinic system with P21/c space group. The compound shows good photo-luminescence property in methanol medium. This Zn(II) complex has been evaluated as a catalytic system in the catalytic oxidation of 3,5-di-tert-butylcatechol (DTBC) in methanol. The Zn(II) complex displays good catecholase like activity with significant turn over, kcat(h–1)=7.99×102 in methanol under aerobic condition. Very interestingly, we are able to isolate the oxidation product as 3,5-di-tert-butylquinone (2) in association with the substrate in the form of a single crystal. Electron paramagnetic resonance (EPR), electron spray ionization (ESI) mass and 1H nuclear magnetic resonance (NMR) spectral analyses of the reaction mixture between Zn(II) complex and DTBC recommend that the course of catalysis proceeds through substrate-catalyst adduct formation & confirm the presence of radical pathways in favour of oxidation products. The computation studies have been executed with density functional theory and all experimental observations are well rationalised with extensive theoretical calculations. Being a redox inactive metal ion, catalytic oxidation of DTBC by Zn(II) complexes will always be a remarkable example in the scientific community.
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