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Title:	An Oxido-Bridged Diiron(II) Complex as Functional Model of Catechol Dioxygenase
Authors:	Yadav, H.R. (/jspui/browse?type=author&value=Yadav%2C+H.R.) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Iron Synthesis X-ray structure Catechol Dioxygenase activity
Issue Date:	2016
Publisher:	Wiley-Blackwell
Citation:	ChemistrySelect, 1(9), pp. 1910-1916
Abstract:	<p>An oxido-bridged diiron(II)-phenanthroline complex, [Fe₂O(phen)₂Cl₂] (1) [phen = 1,10-phenanthroline] has been synthesized from an oxido-bridged diiron(III) precursor in presence of sodium azide and structurally characterized by different spectroscopic tools including single crystal X-ray diffraction study. From X-ray crystal structure of 1, it is revealed that each of the Fe(II) centre is in distorted octahedral geometry with FeN₄OCl core and the molecule crystallizes in Pnc₂ space group. Bond valence sum (BVS) calculation confirms the existence of iron ions in +2 oxidation state in 1. The diiron(II) complex has been evaluated as model system for the catechol dioxygenase enzyme by using 3,5-di-tert-butylcatechol (DTBC) as the substrate in acetonitrile medium, revealing that 1 efficiently mimics the catalytic cycle of catechol dioxygenase. Upon stoichiometric addition of DTBC pretreated with two equivalents of triethylamine (Et₃N) to the diiron complex, two catecholate-to-iron(III) LMCT bands (515 nm and 734 nm) are observed. The in situ generated catecholate adduct from 1 in acetonitrile solution react with dioxygen to afford exclusively extradiol cleavage products along with a small amount of benzoquinone, which is also discerned from the appearance and decrease in intensity of the electronic spectral bands around (708 nm; 507 nm) nm. Nucleophilic attack by molecular oxygen on catecholate adduct in solution provides substantial evidence for the regioselective extradiol cleavage products.</p>
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