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Title:	Catalytic promiscuity of an iron(II)–phenanthroline complex
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:	Activity iron(II) X-ray structure Catecholase activity Catechol dioxygenase Phenanthroline
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Publisher:	John Wiley & Sons, Ltd.
Citation:	Applied Organometallic Chemistry, 31(1).
Abstract:	<p>A mononuclear iron(II) complex, [Fe(phen)₃]Cl₂ (1) (phen = 1,10-phenanthroline), has been synthesized in crystalline phase and characterized using various spectroscopic techniques including single crystal X-ray diffraction. Crystal structure analysis revealed that 1 crystallizes in a monoclinic system with C₂/m space group. Complex 1 acts as a functional model for a biomimetic catalyst promoting the aerobic oxidation of 3,5-di-tert-butylcatechol (3,5-DTBC) through radical pathways with a significant turnover number ($k_{cat} = 3.55 \times 10^3 \text{ h}^{-1}$) and exhibits catechol dioxygenase activity towards the same 3,5-DTBC substrate at room temperature in oxygen-saturated ethanol medium. The existence of an isobestic point at 610 nm from spectrophotometric data indicates the presence of Fe³⁺–3,5-DTBC adduct favouring an enzyme–substrate binding phenomenon. Upon stoichiometric addition of 3,5-DTBC pretreated with two equivalents of triethylamine to the iron complex, two catecholate-to-iron(III) ligand-to-metal charge transfer bands (575 and 721 nm) are observed and the in situ generated catecholate intermediate reacts with dioxygen ($k_{obs} = 9.89 \times 10^{-4} \text{ min}^{-1}$) in ethanol medium to afford exclusively intradiol cleavage products along with a small amount of benzoquinone, and a small amount of extradiol cleavage products, which provide substantial evidence for a substrate activation mechanism. Copyright © 2016 John Wiley & Sons, Ltd.</p>
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