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Title:	Biomimics of phenazine oxidase activity of a cobalt (III)-dipyridylamine complex: Spectroscopic structural and computational studies
Authors:	Joshi, Mayank (/jspui/browse?type=author&value=Joshi%2C+Mayank) Choudhury, Angshuman Roy (/jspui/browse?type=author&value=Choudhury%2C+Angshuman+Roy)
Keywords:	Crystal Engineering Density Functional Theory
Issue Date:	2022
Publisher:	Wiley
Citation:	Applied Organometallic Chemistry, 36(1), 6483
Abstract:	<p>This manuscript demonstrates the synthesis, structural characterization, computational studies, and biomimics of the phenazine oxidase activity of a newly designed cobalt (III) complex, [Co(dpa)(dpa-H+)(N3)2]Cl2 (1) [dpa = 2,2'-dipyridylamine] under an aerobic condition. The crystal structure analysis reveals that the cobalt (III) center adopts an octahedral geometry, and the complex forms a beautiful supramolecular framework through noncovalent interactions. The cobalt (III) catalyst turns out to be a promising catalyst for the oxidative coupling of o-phenylenediamine (OPD) in oxygen-saturated methanol with an excellent turnover number, <math>k_{cat} = 7.85 \times 10^3 \text{ h}^{-1}</math>. Spectrophotometric, electrochemical, mass spectrometry, and computational analysis ensure that the course of catalysis undergoes through a catalyst-substrate complexation, facilitating the development of cobalt-iminobenzoquinone species in the solution. The computational calculations employing the density functional theory (DFT) throw a light to the mechanistic insights of the phenazine oxidase mimics. ETS-NOCV (extended transition state-natural orbitals for chemical valence) plots of the reactive intermediates portray the coordination-driven depletion of electron density from the nitrogens of OPD to cobalt center leading to the enhancement of electrophilic character on para-positioned C-atoms with respect to N-atoms of OPD, thereby catalyzing the nucleophilic attack by second OPD to produce the oxidation product, 2,3-diaminophenazine (DAP). Interestingly, we are able to isolate the oxidation product of the OPD oxidation reaction as a hydrated chloride salt, <math>\text{DAPH}^+\text{Cl}^- \cdot 3\text{H}_2\text{O}</math> (2). The crystal engineering perspectives of 2 attribute the intriguing fate of the secondary chlorides for the stabilization of the oxidation product in crystalline phase.</p>
Description:	Only IISER Mohali authors are available in the record.
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