



# Library Indian Institute of Science Education and Research Mohali



**DSpace@IISERMohali (/jspui/)**  
**/ Publications of IISER Mohali (/jspui/handle/123456789/4)**  
**/ Research Articles (/jspui/handle/123456789/9)**

Please use this identifier to cite or link to this item: <http://hdl.handle.net/123456789/1651>


Title:	Phenoxazinone synthase and antimicrobial activity by a bis(1,3-diamino-2-propanolate) cobalt(III) complex
Authors:	Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Bio-mimicking Chemistry Cobalt(III) DFT study Phenoxazinone synthase activity X-ray structure
Issue Date:	2018
Publisher:	Springer Link
Citation:	Journal of Chemical Sciences, 130(12)
Abstract:	<p>In this work, we have synthesised and structurally characterized a mononuclear cobalt(III) complex, <math>[\text{Co}(\text{2-O-pn})_2]\text{Cl} \cdot 2\text{H}_2\text{O}</math> (1), (2-O-pn = 1,3-diamino-2-propanolate). From the X-ray structure of the cobalt complex, it is revealed that Co(III) ion in 1 adopts an octahedral geometry and crystallizes in the monoclinic system with <math>\text{C2/c}</math> space group. The lattice aqua molecule in combination with chloride ion in 1 forms a water-chloride cluster, <math>(\text{H}_2\text{O})_2 \cdots (\text{Cl})_2</math> through strong H-bonding interaction mediated via cobalt(III) complex in a unique binding motif. This cobalt(III) complex has been tested as an effective catalytic system towards the oxidative coupling of 2-aminophenol (2-AP) in the MeCN medium. In situ mass spectral analysis confirms that 2-AP forms an adduct with cobalt ion and the course of catalysis proceeds through catalyst-substrate binding followed by oxidative coupling of 2-AP with iminobenzoquinone. This cobalt(III) catalyst affords exclusively aminophenoxazinone species with a significant turnover number, <math>k_{\text{cat}}: 6.37 \times 10^2 \text{h}^{-1}</math> in the MeCN medium. This cobalt(III) complex is able to screen out the growth of some bacteria and fungi species. Quantum chemical calculations employing density functional theory is used to model structural parameters and spectroscopic behaviour. The theoretical findings corroborate well with the experimental results.</p>
Description:	Only IISERM authors are available in the record.
URI:	<a href="https://link.springer.com/article/10.1007/s12039-018-1562-9">https://link.springer.com/article/10.1007/s12039-018-1562-9</a> ( <a href="https://link.springer.com/article/10.1007/s12039-018-1562-9">https://link.springer.com/article/10.1007/s12039-018-1562-9</a> ) <a href="http://hdl.handle.net/123456789/1651">http://hdl.handle.net/123456789/1651</a> ( <a href="http://hdl.handle.net/123456789/1651">http://hdl.handle.net/123456789/1651</a> )
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

## Files in This Item:

File	Description	Size	Format
Need to add pdf.odt (/jspui/bitstream/123456789/1651/1/Need%20to%20add%20pdf.odt)		8.04 kB	OpenDocument Text

[View/Open \(/jspui/bitstream/123456789/1651/1/Need%20to%20add%20pdf.odt\)](#)

Show full item record (</jspui/handle/123456789/1651?mode=full>)

 (</jspui/handle/123456789/1651/statistics>)

Items in DSpace are protected by copyright, with all rights reserved, unless otherwise indicated.