Title:	Synthesis and structural characterization of a linkage isomer to a mononuclear Nickel(II) complex: Experimental and computational depiction of phosphoesterase efficiency☆
Authors:	Joshi, Mayank (/jspui/browse?type=author&value=Joshi%2C+Mayank) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Bio-mimicking chemistry DFT study Linkage isomer Nickel(II)Phosphatase activity X-ray structure
Issue Date:	2020
Publisher:	Elsevier
Citation:	Journal of Molecular Structure 1200,127083
Abstract:	Synthesis and structural characterization of a linkage isomer, bis(2,2′-dipyridylamine)dithiocyanato(k-S)nickel(II), [Ni(dpa)2(k-SCN)2] (1) of a previously reported Ni(II) complex, [Ni(dpa)2(k-NCS)2] (dpa = 2,2′-dipyridylamine; SCN = thiocyanate) has been reported herein. X-ray structural analysis of 1 reveals that Ni(II) complex crystallizes in monoclinic system with P21/c space group and exists in trans configuration. The coordination geometry for 1 adopts a tetragonal structure. Supramolecular aspects of the Ni(II) complex indicate that N atom of SCN behaves as a donor and H atom of dpa ligand acts as a receptor in growing 1D crystalline structure along b axis in solid state. The aromatic rings in 1 prefer to exist in face-centred stacking with interplanar distance of 3.426 Å and supports strongly to form self-assembled 3D crystalline architecture. Hirshfeld surface analysis further recommends this crystalline assembly in solid state. 1 exhibits promising phosphatase activity towards disodium(4-nitrophenyl)phosphate (PNPP) in aqueous-methanolic medium. The hydrolytic phosphatase efficiency for 1 is determined in terms of turnover number (kcat) as 3.38 × 104 h−1. Moreover, density functional theoretical computations closely replicate the structural parameters and spectroscopic behaviour of 1.
Description:	Only IISERM authors are available in the record.
URI:	https://www.sciencedirect.com/science/article/pii/S0022286019311834?via%3Dihub (https://www.sciencedirect.com/science/article/pii/S0022286019311834?via%3Dihub) http://hdl.handle.net/123456789/3422 (http://hdl.handle.net/123456789/3422)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/3422/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/3422?mode=full)

(/jspui/handle/123456789/3422/statistics)