



Experimental and computational studies of di- μ -chlorido-bis[chlorido(1,10-phenanthroline- K^2N,N')nickel(II)] $NiCl_2(H_2O)(C_{12}N_2H_8)$: Crystal structure, quantitative analysis of the intermolecular interactions and electronic properties

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ARTICLE INFO

Article history:

Received 2 September 2020

Revised 31 October 2020

Accepted 2 November 2020

Available online 3 November 2020

Keywords:

Ni(II) complex

Crystal structure

Hirshfeld surface analysis

MEP map

Quantum chemical calculations

ABSTRACT

$NiCl_2(H_2O)(C_{12}N_2H_8)$ was synthesized in solution and its structure was studied by single-crystal X-ray diffraction. It crystallizes in the monoclinic system (S. G.: $P2_1/n$), $Z = 4$, with the cell parameters (\AA , $^\circ$): $a = 12.6640(5)$, $b = 6.8322(3)$, $c = 14.2054(5)$ and $\beta = 93.569(3)$. The final residual factors of the refined structure model R/R_w were 0.031/0.082 for 2156 independent reflexions and 172 parameters. The crystal structure is described in terms of $Ni_2Cl_4(H_2O)_2(Phen)_2$ dimmers interacting through weak intermolecular O–H...Cl Hydrogen bonds. The 2D fingerprint plots, built using the Hirshfeld surface analysis, helped analyzing and quantifying all the intermolecular contacts and revealed the main intermolecular interactions around the title complex. The computational investigation was undertaken at M06–2X/6–31G(d)(LANL2DZ) level by using Gaussian.

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1. Introduction

The molecule 1,10-phenanthroline (**Phen**) and its different derivatives are considered as interesting ligands used in various chemical industries [1]. Heteroatomic group of Phen provides a binding site for different metal ions. It has a rigid structure and has two aromatic nitrogen atoms which contain unshared electronic pairs that can bind metals [2,3]. Due to its electron deficiency, Phen turns to be a good acceptor leading then to various applications such as catalysis, redox, photo-redox and biological activities [3–8]. Especially in supramolecular chemistry, Phen derivatives are reported to play a key role [9–11].

Metal complexes with 5-amino-1,10-phenanthroline (**aphen**) were reported to be interesting potentiometric sensors, $M^{+2} = 3d$ transition metal, including Zn [12]. Moreover, Tammiku et al. reported that the complexation of magnesium halide MgX_2 with

Phen is the reason for the disappearance of the red color of the complex $RMgX(phen)$ near the titration end point [13]. The anticancer properties of the lanthanum compound [tris(1,10-phenanthroline)lanthanum(III)] triithiocyanate have been published by Heffeter et al. [14]. Recently, photochemical properties of a series of 1,10-phenanthroline complexes have been reported [15]. Since phen is considered as a classic ligand used in coordination chemistry, which couples versatility in metal ion binding with atypical properties of its complexes, Phen-based metal complexes can interact with DNA in an intercalative fashion inducing, in some cases, DNA cleavage [16]. However, even with this last ability, molecular phen could not be medically used, due to its toxicity caused by inhibiting metalloenzymes via its chelating nitrogen atoms. Nonetheless, the toxicity has been bypassed for its attractive features coordinating with transition metals [17]. Alreja and Kaur published a review of the developments of phen ligands behaving as chemosensors for anions and cations. Their investigations yielded a database of various phen-derived receptors serving as chemosensors for various analytes

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