



Structural investigations, Hirshfeld surface analyses, and molecular docking studies of a phenoxo-bridged binuclear Zinc(II) complex



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ABSTRACT

A novel phenoxo-bridged zinc complex, $[Zn_2(L)\mu(O-O)_2H_2OCl_2]$ [L= deprotonated salen ligand, 2,2'-((1E,1'E)-((2,2-dimethylpropane-1,3-diyl)bis(azanelylidene))bis(methaneylylidene)diphenol)], was reported. The title complex was characterized by elemental analyses, single crystal X-ray crystallography, spectroscopic studies, and thermogravimetric analysis. The X-ray structure analysis reveals the coordination of Zn₁ atom to two imine nitrogen atoms, two phenolic oxygen atoms, and the oxygen atom of aqua ligand, giving it a distorted square pyramidal geometry, whereas the Zn₂ atom is bonded to the same phenoxide anions, and two chloride ions, resulting in a distorted tetrahedral geometry. In addition, TD-DFT and NBO analyses were investigated to obtain bonding information insights into the structure. Furthermore, Hirshfeld surface analysis was used to determine various intermolecular interactions in the complex. Furthermore, a docking analysis was performed on the B-DNA [sequence d(CGCGAATTCGCG)₂dodecamer] (PDB ID:1BNA) using the AutoDockvina (scripps) software package. The fluorescence property of the title complex was also carried out, and revealed it to be excellent photoluminescent material.

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1. Introduction

Coordination compounds with 3d transition metal ions have recently gained a lot of interest for their crucial roles in the chemistry of metallo-enzymes, biology and material science because of their widespread availability and low cost [1–3]. Zinc, one of most important bio-metals in nature, has excellent opto-electronic, luminous, biological, and catalytic properties, making it one of the most intriguing candidate in the field of advanced materials [4–7]. Enzymes having more than one zinc atom in the active site, such as phospholipase C (PLC) and nuclease P1(NPI), have attracted lot attention in recent years [8]. In the active site, crystal structural analysis reveals three zinc atoms, two of which are joined by a bridging hydroxide group or water molecule, and a third carboxylate functional groups [8]. Transition metal complexes containing

oxygen and nitrogen donor Schiff bases are widely used as functional materials because of their interesting topology, structural lability, and sensitivity to molecular environments [9–11]. Furthermore, Schiff bases with diverse coordination modes may encapsulate large number of metal ions, allowing for the successful synthesis of several coordination compounds with wide range of stereochemistry [9–12]. However, among the various Schiff bases, salen-type Schiff bases have been reported to form their metal complexes with unique coordination, high thermodynamic stability, and kinetic inertness [12–14]. In addition, size of the metal ion influences the geometry of the metal complexes, the intrinsic stiffness of the ligand due to the presence of aromatic rings and repulsion between various atoms [15,16]. In literature, the deprotonated salen ligands or its related derivate as an ONNO tetradentate chelating ligand are known to form polynuclear complexes [17,18]. Furthermore, a ligand with similar characteristics has also been reported to produce mononuclear complexes in literature [19–22]. Moreover, phenoxide anion of the salen ligand can form binuclear complexes by bridging another metal ion [23,24]. They can also

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