



A bowl-shaped phenoxido-bridged binuclear zinc complex: Experimental and theoretical studies

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ABSTRACT

A new dinuclear zinc coordination complex with di(μ -alkoxido) bridge obtained from $[[H_2L = N,N$ -(salicyaldene)-1,3-diaminopropan-2-ol]] was investigated by IR, 1H - & ^{13}C NMR spectroscopy. Single crystal X-ray analysis reveals that the Zn1 atom in the title complex is five coordinated and bound to two alkoxide atoms, two nitrogen atoms, and a chloride ion at apical position in distorted square pyramid geometry, while the second central cation, Zn2, is four coordinated and its O2Cl2 coordination environment is distorted tetrahedral. The single-crystal X-ray crystallographic measurements and DFT calculations reveal that the complex has a bowl-like structure. Hirshfeld surface analysis, energy frameworks QTAIM, NBO, and EDA analyses show clearly that the structure contains a variety of classical and non-classical interactions that help to extend the crystal net dimension. TGA is used to investigate the stability of the structure of the title complex.

1. Introduction

Multifunctional ligands and their complexes with transition metal ions, especially 3d metal ions, have become increasingly important in recent years due to their low cost and easy accessibility, as well as their wide range of applications as functional materials in material science and intriguing topologies [1,2]. In recent years, there has been a lot of interest in the chemistry of polynuclear metal complexes and their use in catalysis, as well as the development of new functional materials [3]. The well-designed polydentate ligands are ubiquitous in coordination chemistry because of the beautiful architecture of polynuclear complexes [3]. Transition metal complexes with O, N possessing Schiff bases are widely used in coordination owing to their fascinating structures, lability, and various denticity [4,5]. There are also many reports in the literature about the bridging of the phenolate oxygen atoms of Salen type Schiff bases as candidates for forming complexes with beautiful topology [6–9]. Zinc, a redox-active metal ion, is the second most common bio-relevant trace metal in humans after iron, with important properties in catalysis, photoluminescence, biology, and materials science [10–12]. Enzymes with multinuclear zinc atoms in the active site,

typically at the distorted polyhedral, and a labile ligand, such as water, have attracted a lot of attention in recent decades [13,14]. Furthermore, Zn(II) coordination complexes are versatile candidates because of their roles in catalysis, metalloenzymes, photoactive materials, material science, and various biological applications, such as antimicrobial, antibacterial, and antidiabetics [15–19]. In addition, Zn(II) complexes are also good candidates for designing metalodrugs, particularly anticancer drugs, because of their low toxicity and low propensity to change oxidation states [20,21]. The Schiff base ligand N, N'-bis(salicylidene)-1,3-diaminopropan-2-ol (H_3L) with five donor atoms, which produces μ -alkoxido bridged complexes, is of great importance in coordination chemistry because of its variable denticity [22–24]. Furthermore, there have been several reports of binuclear zinc complexes with intriguing architectures containing salen ligands and their applications in material and biological sciences [25–29]. There are many reports in the literature of the use of N,N'-bis(salicylidene)-1,3-diaminopropan-2-ol (H_3L) in the construction of various coordination complexes with surprising topologies, such as the formation of trinuclear zinc(II) complexes, dinuclear Fe(III) complexes, tetranuclear manganese, and Co(III) complexes, binuclear copper(II) complexes,

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