



Synthesis, characterization and X-ray crystal structure of a mononuclear ampyrone based zinc complex

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ABSTRACT

A novel mononuclear zinc complex derived from a pyrazole-based ligand was studied. The structure of the complex was explored using C, H, N, FT-IR, NMR, and UV/Vis studies, thermogravimetric analysis, and single-crystal X-ray crystallography. The single XRD study shows the coordination of the zinc ion to the alkoxide oxygen atom, two chloride ions, and one additional oxygen atom from the ethanol molecule in the complex. The intermolecular interactions in the complex were investigated using Hirshfeld surface analysis and revealed that the H...H is the most important interaction, accounting for 45.9% of the overall crystal packing contribution of the complex.

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1. Introduction

4-Aminoantipyrine (4-AAP), a derivative of pyrazole with two adjacent nitrogen atoms embedded in its ring and attached to a reactive amino group and a carbonyl functional group, is very important pharmaceutical component, and plays a key role in bioinorganic chemistry, coordination chemistry, and several biological systems [1–3]. In addition, this organic scaffold has also been used for the synthesis of dihydrotestosterone products [5]. Furthermore, 4-aminoantipyrine and its derivatives also show antioxidant, anticancer, antimicrobial, anti-TB, anti-HIV, and catalytic properties [6–8]. The amino group of 4-aminoantipyrine is extremely reactive at ambient temperature, and interacts quickly with ketones and aldehydes. As a result, it's commonly used as a nitrogen scavenger species to combat hydroxyl radicals [9]. Furthermore, the presence of hetero atoms affects electron re-distribution and thus exhibits aromatic character, known as heteroatom effect [10], which confers reactivity, chelating and other properties. As a result, it is used in wide range of research areas, including analytical, modern organic, bioorganic, and medicinal chemistry [11,12].

Azomethine derivatives of 4-AAP obtained by the condensation reaction of amino/carbonyl group of the 4-AAP scaffold with another organic scaffold bearing aldehyde/keto or amino group, yielding multiple donor sites, have received huge attention over the years and played an extensive role in catalysis, dyes, material chemistry, analytical and medicinal chemistry [13–19]. Furthermore, the presence of sp^2 hybrid orbital of nitrogen atom of imine linkage make them excellent donor ligands. Moreover, the chelating abilities of the Schiff bases escalate when the number of donor atoms in the vicinity of the imine linkage increases [20]. Therefore, the chelating properties of Schiff bases comprising 4-AAP have drawn a lot of attention from the researcher due to the presence of potential donor sites, resulting in the formation of three types of complexes with metal ion [14], namely (i) complexes using both the donor atoms, (ii) amine salts utilizing only the amino nitrogen atoms, and (iii) complexes utilizing only the carbonyl oxygen atom or amino nitrogen atom in coordination [21–23].

Considering the vast significance of 4-AAP and its derivatives [1–5], we are here interested to design a new zinc complex produced from ampyrone based ligand, HL, 4-[(1-Hydroxy-2-naphthyl)methyl-ene-amino]-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one, synthesized by the condensation of 2-hydroxynaphthaldehyde and 4-AAP [24]. Elemental analysis, FT-IR, NMR, MS, UV/Vis and single crystal X-ray crystallography were used to characterize the

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