

Novel Nickel(II) Complex With A Thiosemicarbazide: Synthesis, Structure And Noncovalent Interactions

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Thiosemicarbazides research has shown the great potential of these compounds as antimicrobial, antifungicide, and antitumor agents [1,2]. A few drugs like triapine, amithiozone and marboran have proven efficiency studies against diseases, and all these chemical compounds belong to the thiosemicarbazide group [3]. Therefore, this class of organic ligands caught the attention of bioinorganic chemistry due to its ability to coordinate with transition metals [4]. This coordination is characterized by the basic regions of the ligand and the acidic metal center, which may potentiate pharmacological activity [5]. Nickel plays an important role in the biology of microorganisms and macroorganisms [6]. Nickel(II) with thiosemicarbazides complexes have received attention due to identifying a sulfur-rich coordination environment in biological nickel centers, such as the active sites of certain ureases and hydrogenases [7]. This present work reports the synthesis, crystal structure, and investigation of noncovalent interactions of new nickel(II) complex, $[\text{Ni}(\text{ptsc})_3]\text{Cl}_2 \cdot 2\text{H}_2\text{O}(\text{DMF})$ with 4- phenylthiosemicarbazide ligand (ptsc). The synthesis of the complex was carried out in acetonitrile and the blue solid obtained from the mother solution was recrystallized in DMF with a yield of 89%. The crystals were investigated by single crystal X-ray analysis, Hirshfeld surface, physicochemical and spectroscopic methods. The single-crystal X-ray study reveals three thiosemicarbazide molecules coordinated bidentate through the NS-donor atoms and resulted in distorted octahedral geometry with the nickel atom, Figure 1. The crystal structure of the complex is stabilized by noncovalent interactions, such as hydrogen bonds and van der Waals interactions, as observed in Figure 2. The intermolecular interactions of the complexes were quantitatively analyzed by 3D Hirshfeld surface and associated 2D fingerprint plots.

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References:

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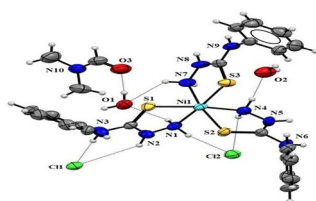


Figure 1. Molecular structure of $[\text{Ni}(\text{tsc})_3]\text{Cl}_2 \cdot 2\text{H}_2\text{O}(\text{DMF})$ showing intermolecular hydrogen interactions (dotted lines).

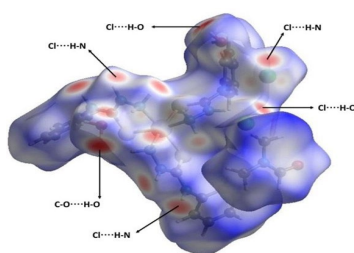


Figure 2. Hirshfeld surface mapped with d_{norm} of the complex $[\text{Ni}(\text{tsc})_3]\text{Cl}_2 \cdot 2\text{H}_2\text{O}(\text{DMF})$.