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# Synthesis, structure, physicochemical characterization and theoretical evaluation of non-covalent interaction energy of a polymeric copper(II)-hydrazone complex

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## Abstract

One dimensional polymeric copper-hydrazone complex  $\{[\text{Cu}(\text{H}_{0.5}\text{L})(\mu_{1,3}\text{-SCN})]0.5\text{ClO}_4 \cdot 0.5\text{MeOH}\}_n$  (**1**) has been synthesized with  $\text{Cu}(\text{ClO}_4)_2 \cdot x\text{H}_2\text{O}$  and  $N'$ -(1-(pyridin-2-yl)ethylidene)acetohydrazide (HL) in presence of NaSCN. The ligand and the complex have been characterized by several spectroscopic techniques (IR, UV-Vis and EPR), cyclic voltammetry and the structure of **1** has been determined by single crystal X-ray diffraction. The complex is an infinite one dimensional polymer bridged by thiocyanate. The magneto-structural correlation has been determined and the non-covalent interactions present in the molecule have been energetically evaluated by means of DFT calculations.

**Keywords:** Copper(II)-hydrazone complex; 1D chain; H-bonds; Antiferromagnetism;  $\pi$ -hole interaction; MEP analysis.

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