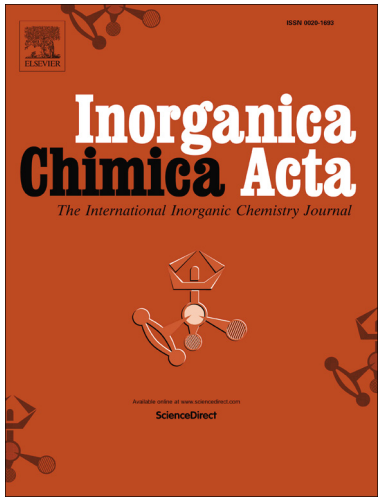

Research paper

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PII: S0020-1693(18)30002-1
DOI: https://doi.org/10.1016/j.ica.2018.09.031
Reference: ICA 18489

To appear in: *Inorganica Chimica Acta*

Received Date: 1 January 2018
Revised Date: 31 July 2018
Accepted Date: 9 September 2018

Please cite this article as: D. Sadhukhan, M. Maiti, A. Bauzá, A. Frontera, E. Garribba, C.J. Gomez-García, Synthesis, structure, physicochemical characterization and theoretical evaluation of non-covalent interaction energy of a polymeric copper(II)-hydrazone complex, *Inorganica Chimica Acta* (2018), doi: https://doi.org/10.1016/j.ica.2018.09.031

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 $\{[Cu(H_{0.5}L)(\mu_{1,3}\text{-}SCN)]0.5ClO_4.0.5MeOH\}_n$ (**1**) has been synthesized with $Cu(ClO_4)_2{\cdot}xH_2O$ 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; π-hole interaction; MEP analysis.