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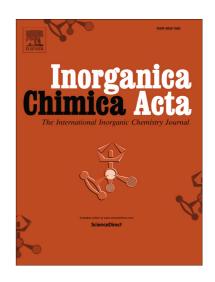
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ACCEPTED MANUSCRIPT

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

Dipali Sadhukhan*^{a,b}, Monami Maiti^{a,c}, Antonio Bauzá^d, Antonio Frontera^d, Eugenio Garribba^e, Carlos J. Gomez-García^f

^aDepartment of Chemistry, Jadavpur University, Kolkata 700032, India ^bCurrent affiliation: Centre de Recherche Paul Pascal (CRPP), 115 Avenue du Dr. A. Schweitzer, Pessac 33600, France

^cCurrent affiliation: Department of Chemistry, Narasinha Dutt College, Howrah, West Bengal, India

^dDepartament de Química, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma de Mallorca (Balears), Spain

^eDipartimento di Chimica e Farmacia, Università di Sassari, Via Vienna 2, I-07100 Sassari, Italy

^fInstituto de Ciencia Molecular (ICMol), Dpto. Química Inorgánica. Universidad de Valencia, 46980 Paterna, Spain

*Corresponding author. Tel.: +33 758715798, Email: dipali@crpp-bordeaux.cnrs.fr

Abstract

One dimensional polymeric copper-hydrazone complex $\{[Cu(H_{0.5}L)(\mu_{I,3}-SCN)]0.5ClO_4.0.5MeOH\}_n$ (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.

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