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# Magnetic Ordering of three Thiosemicarbazonecopper(II) Complexes

During the last decades, metal-organic compounds constitute an active field of research, and among them, complexes that combine thiosemicarbazone ligands with copper(II) are appealing from the point of view of material science due to their interesting structural and magnetic properties [1]. Complementary, they are also extensively studied due to biological and pharmacological applications that rely on their rich coordination and redox chemistry [2].

We present a first principles study of three thiosemicarbazone copper complexes: [{CuLX}2], with X=Cl, Br and I (Fig. 1). All of them crystallize in isomorphous triclinic structures that contain one dimer per unit cell [3,4]. In order to study their magnetic structure, we have calculated the energies for the ferromagnetic and all the antiferromagnetic orderings compatible with a supercell containing 2×2×2 crystallographic unit cells (Fig. 2). Results show that energy differences between the most stable structures for each X halide are very small (several meV/dimer/), and as a consequence, the ground state cannot be assigned unambiguously to a single ordering, any of the low energy structures being a valid candidate for the ground state.

We have also evaluated the magnetic exchange interactions by mapping the calculated energies of all the magnetic orderings to the Ising model taking into account couplings between the first and second neighbours. It can be concluded that the competition between ferro/antiferro and intra/interdimeric interactions is the origin of the complex magnetic energy landscape present in these materials.

[1] J. García-Tojal, R. Gil-García, P. Gómez-Saiz, M. Ugalde, Curr. Inorg. Chem., 1, 189 (2011).

[2] T. S. Lobana, R. Sharma, G. Bawa, S. Khanna, Coord. Chem. Rev., 253, 977 (2009).

[3] P. Gómez-Saiz, J. García-Tojal, M. A. Maestro, J. Mahía, F. J. Arnaiz, L. Lezama, T. Rojo, Eur. J. Inorg. Chem., 2639 (2003).

[4] J. García-Tojal, M. K. Urtiaga, R. Cortes, L. Lezama, M. I. Arriortua, T. Rojo, J. Chem. Soc., Dalton Trans., 2233 (1994).

## Summary

## Topic

1. Electrons and spins

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