2005 Vol.43 No.2 pp.349-352 DOI:

Strong Ferromagnetic Coupling of $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ with Simultaneous End-on Azido and Carboxylato Bridges: a First Principle Study

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(Received: 2004-3-2; Revised:)

Abstract: The compound $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ (Hpht=hydrogen phthalate) is formed by chains of copper atoms bridged simultaneously by syn-syn carboxylato and end-on azido bridges. Taking into account the large Cu-O(1)-C(7) bond angle of the single carboxylato bridge (131º), or the large Cu-N(11)-Cu bond angle of the azido bridge (111.9º), a moderately intrachain antiferromagnetic behavior should be expected for the compound. This paper is devoted to examining the apparently anomalous intrachain ferromagnetic behavior of $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$, using first principles within the full potential linearized augmented plane wave (FP-LAPW) method. The total energy, the density of states (DOS), and the spin distributions are obtained. The atomic spin distribution has been analyzed as resulting from the interplay of electron delocalization and spin polarization. The DOS reveals a surprisingly strong exchange interaction between the d type orbitals of the copper and the π molecular orbitals of the two ligands.

PACS: 75.30.Et, 71.20.-b, 61.82.Pv, 71.15.Mb

Key words: ferromagnetic coupling, spin polarization, superexchange interaction

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