

H-bonded supramolecular synthon induced magnetic superexchange phenomenon results weak ferromagnetic and strong antiferromagnetic interactions in two new copper-orotate coordination network.

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Streszczenie

Hydrothermal self-assembly of orotic acid ($C_5H_4N_2O_4$ double bond; length as m -dashOrH3) with metal salt $Cu(Ac)_2 \cdot H_2O$ yielded a new OrH based hydrogen bonded coordination network of formula $[Cu(OrH)(2NH_3)(H_2O)] \cdot H_2O$ (1) and $[Cu(OrH)(2NH_3)]_2$ (2). Single crystal X-ray study on 1 confirms that +2 charges on the metal ions (Cu^{2+}) are balanced by OrH anion. $N-H \cdots O$ and $O-H \cdots O$ hydrogen bonding synthons are the only artifact for the resulting hydrogen bonded copper-OrH architecture. Temperature dependent measurements of magnetic susceptibility reveals the occurrence of competitive exchange interactions with a net ferromagnetic character in 1 ($J = +0.48 \text{ cm}^{-1}$) and strong antiferromagnetic interaction in 2 ($J = -4.93 \text{ cm}^{-1}$). Magnetic superexchange interaction transmitted through equatorial-axial hydrogen bridge system promotes weak ferromagnetic interactions in 1 while in 2 it is in basal-basal position, in which two dx^2-y^2 orbitals is involved in exchange mechanism reveals the coexistence of two antiferromagnetic exchange pathways, intramolecular much stronger than intermolecular. The natural bond orbital (NBO) analysis applied separately to α and β spin density matrices clearly shows two important magnetic superexchange pathway with shorter $Cu \cdots Cu$ contact $5.542(4) \text{ \AA}$ and $4.845(4) \text{ \AA}$ or $5.755(1) \text{ \AA}$ in (1) and inter dimer $6.665(1) \text{ \AA}$ and $4.6744(9) \text{ \AA}$ for (2).

Słowa kluczowe

Hydrogen bonding, Metal-OrH coordination network, Ferromagnetic and antiferromagnetic interactions, DFT calculation

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