

Crystal structure and magnetic interactions of a new alkoxido and azido bridged 1D copper(II) coordination polymer.

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A new 1D azido and alkoxido-bridged Cu(II) coordination polymer, $[\text{Cu}_2(\text{H}_3\text{L})(\mu\text{-H}_2\text{L})(\mu\text{-N}_3)]_n$ (1), was synthesized from the reaction of H_4L , $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ and NaN_3 in methanol, where H_4L is (*E*)-2-((5-bromo-2-hydroxybenzylidene)amino)-2-(hydroxymethyl)propane-1,3-diol. Compound 1 was characterized by elemental analysis, spectroscopic methods and single-crystal X-ray diffraction. Both spectroscopic and structural studies confirmed the presence of the Schiff base and the azide ligands. Azido and alkoxido bridges connect two Cu(II) ions with different coordination environments. The Schiff base ligand, H_4L , shows two coordination modes acting as H_3L^- and H_2L^{2-} to the metal cores. The azido ligands show both end-on and end-to-end bridging modes. The magnetic study performed in the 1.8–300 K range shows an overall ferromagnetic interaction among the copper(II) ions dominated by the coupling through the alkoxido bridge. We have calculated the value of the magnetic coupling constants by means of DFT calculations, and we compared their values with those obtained from the magnetic susceptibility measurements.

Słowa kluczowe

Magnetic interaction, Coordination polymer, Crystal structure, DFT calculation, Copper

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