X-ray crystal structures, electron paramagnetic resonance, and magnetic studies on strongly antiferromagnetically coupled mixed μ-hydroxide-μ-N^1,N^2-triazole-bridged one dimensional linear chain copper(II) complexes.

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Streszczenie

Four new metal-organic polymeric complexes, {[Cu(mu-OH)(mu-ClPhtrz)][(H 2O)(BF 4)]} n (1), {[Cu(mu-OH)(mu-BrPhtrz)][(H 2O)(BF 4)]} n (2), {[Cu(mu-OH)(mu-ClPhtrz)(H 2O)](NO 3)} n (3), and {[Cu(mu-OH)(mu-BrPhtrz)(H 2O)](NO 3)} n (4) (ClPhtrz = N-[(E)-(4-chlorophenyl)methylidene]-4 H-1,2,4-triazol-4-amine; BrPhtrz = N-[(E)-(4-bromophenyl)methylidene]-4 H-1,2,4-triazol-4-amine), were synthesized in a reaction of substituted 1,2,4-triazole and various copper(II) salts in water/acetonitrile solutions. The structures of 1- 4 were characterized by single-crystal X-ray diffraction analysis. The Cu(II) ions are linked both by single N (1), N (2)-1,2,4-triazole and hydroxide bridges yielding one dimensional (1D) linear chain polymers. The tetragonally distorted octahedral geometry of copper atoms is completed alternately by two water and two BF 4 (-) anion molecules in 1 and 2 but solely by two water molecules in 3 and 4. Magnetic properties of all complexes were studied by variable temperature magnetic susceptibility measurements. The Cu(II) ions are strongly antiferromagnetically coupled with J = -419(1) cm (-1) (1), -412(2) cm (-1) (2), -391(3) cm (-1) (3), and -608(2) cm (-1) (4) (based on the Hamiltonian H = - J[summation operator S i . S i+ 1]). The nature and the magnitude of the antiferromagnetic exchange were discussed on the basis of complementarity/countercomplementarity of the two competing bridges.

Adres publiczny

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https://www.acs.org/content/acs/en.html