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Synthesis, crystal structure and magnetic properties of a novel copper(II) complex with sulfoisophthalic acid.

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A new Cu(II) complex, $[Cu_2(\mu_2\text{-}OH_2)_2(HSIP)_2(H_2O)_6]$ (H_3SIP = 5-sulfoisophthalic acid), has been synthesized and characterized by single crystal X-ray diffraction, EPR spectroscopy (X- (9.5 GHz) and Q-band (35 GHz)) and magnetic measurements. The solid state structure of the complex consists of coordination dimers $[Cu_2(\mu_2\text{-}OH_2)_2(HSIP)_2(H_2O)_6]$ which are hydrogen bonded into 3D network. The neighbouring metal ions form a rare example of centrosymetric dinuclear core $[Cu_2(\mu_2\text{-}OH_2)_2]$ with equatorial – axial positions of the bridging ligands. The coordination dimers are organized into inorganic monolayers *via* water–sulfonate hydrogen bond intractions, and further linked in 3D structure *via* carboxylic–carboxylic hydrogen bond intractions. The magnetic properties and EPR spectra are discussed in terms of crystal structure features. The X- and Q-band EPR spectra exhibit fine structure signals due to S = 1 and the simulated parameters indicate small zero field splitting parameter D_{exp} ($-0.035\ cm^{-1}$) dominated by D_{dip} ($-0.031\ cm^{-1}$). A usually forbidden $\Delta M_s = 2$ line of lower intensity is observed in the half field region at about 150 mT. The susceptibility data have been analyzed using a spin–ladder model with both ferromagnetic (rungs) and antiferromagnetic (legs) coupling.

Słowa kluczowe

Copper(I) complex, crystal structure, hydrogen-bonded network, EPR Spectra, magnetic properties

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