

Single crystal EPR spectroscopy, magnetic studies and catalytic activity of a self-assembled [2 × 2] Cu^{II}₄ cluster obtained from a carbohydrazone based ligand.

Autorzy

Rahman Bikas

Hassan Hosseini-Monfared

Pavlo Aleshkevych

Ritta Szymczak

Miłosz Siczek

Tadeusz Lis

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Streszczenie

A new tetranuclear [2 × 2] cluster of Cu(II) with a symmetric carbohydrazone based ligand, [Cu₄L₄](NO₃)₄·1.6(H₂O) (**1**), {where HL donates bis-[(E)-N'-(1-(pyridin-2-yl)ethylidene)]carbohydrazide} was synthesized and characterized by spectroscopic methods and X-ray analysis. The EPR spectra were performed on single crystals of complex **1** at various temperatures and allowed the identification and separation of two types of magnetic objects contributing to magnetism: single atoms of Cu(II) and a tetranuclear Cu₄ cluster. The main values of the *g*-factor and hyperfine structure were determined for single ions of Cu(II). The copper atoms in the tetramer are coupled antiferromagnetically with an isotropic antiferromagnetic exchange $J = 215$ K (149.4 cm⁻¹). A small anisotropic exchange of the order of 0.06 K (0.04 cm⁻¹) is responsible for the initial zero-field splitting of the energy levels in the tetramer spectrum. Magnetic measurements of complex **1** confirmed the existence of a strong antiferromagnetic exchange coupling between four Cu(II) ions. Complex **1** showed high potential for the catalytic and selective oxidation of *cis*-cyclooctene with aqueous H₂O₂.

Słowa kluczowe

Single crystal EPR, magnetic studies, Catalytic epoxidation, [2×2] CuII₄ cluster, Exchange coupling

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