

Synthesis, crystal structure and magneto-structural studies of 2D copper(II) coordination polymer containing L-alanine amino acid.

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Streszczenie

A 2D coordination polymer of Cu(II) was synthesized by the reaction of $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ with L-alanine and characterized by elemental analysis, spectroscopic methods and single crystal X-ray studies. X-ray analysis indicated that the compound is a 2D coordination polymer which the carboxylate group of amino acid ligands acts as bridging ligand between Cu(II) ions. The crystal structure of compound is stabilized by intermolecular hydrogen bond interactions. Magnetic susceptibility data of powdered sample between 2 and 300K were interpreted in terms of a 2D-spin model, with weak antiferromagnetic exchange-coupling through *syn-anti* carboxylate bridges, with coupling constant $J = -0.2 \text{ cm}^{-1}$ between nearest-neighbor Cu(II) ions. The results are compared with those obtained from similar studies in other copper amino acid complexes. DFT studies showed that overlap of magnetic $d_{x^2-y^2}$ orbitals of the neighboring Cu(II) ions and the molecular orbitals of bridging carboxylate groups is negligible what makes only weak antiferromagnetic interaction between them. Thermal gravimetric analysis (TGA) indicated that the compound is stable up to 240°C and it converts to CuO at about 800°C . Cyclic voltammetry studies showed a quasi-reversible redox and an irreversible peaks which can be attributed to Cu(I)/Cu(II) and Cu(II)/Cu(III) couples, respectively.

Słowa kluczowe

Cu(II) coordination polymer, magnetic studies, crystal structure, spectroscopic studies, amino acid

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