

Structural and spectroscopic parameters of distortion in $[\text{Cu}(\text{bpy})_2(\text{O}_2\text{SO}_2)]\cdot\text{CH}_3\text{OH}$ and $[\text{Cu}(\text{bpy})_3][\text{SO}_4]\cdot 7.5\text{H}_2\text{O}$: synthesis, crystal structure, spectroscopic and magnetic properties.

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A copper(II) sulfate complex of formula $[\text{Cu}(\text{bpy})_2(\text{O}_2\text{SO}_2)]\text{CH}_3\text{OH}$ (1) (bpy = 2,20-bipyridine) was prepared and characterized by X-ray diffraction, spectroscopic methods (FIR, IR, NIR–Vis–UV, EPR) and magnetic measurement. The S–O distances in the chelating SO_4^{2-} entity give the value of the geometric distortion parameter $D_r = 0.022$. The EPR parameters are temperature dependent and indicated the fluxional model of the $[\text{Cu}(\text{N},\text{N}0)_2\text{OO}]$ chromophore with $d_{x^2-y^2}$ ground state. The electronic spectrum of 1 exhibits the maxima at 9740 and 14 630 cm^{-1} . The very weak antiferromagnetic interaction between copper centers in the crystal lattice was observed. In $[\text{Cu}(\text{bpy})_3][\text{SO}_4]\cdot 7.5\text{H}_2\text{O}$ (2) crystal the distance values in $[\text{Cu}(\text{bpy})_3]^{2+}$ cations result in $T = 0.958$ and the value of D_{rot} of the non-coordinate SO_4^{2-} tetrahedron is 0.095. The value of T for $[\text{CuN}_6]^{2+}$ suggests the fluxional character of Jahn–Teller (JT) distortion supported by the EPR studies. The electronic spectrum shows two separated bands at 6900 and 14 400 cm^{-1} .

Słowa kluczowe

Sulfate(VI) and copper(II) complexes, Geometric distortion, X-ray diffraction, Spectroscopic methods (FIR-IR, NIR–Vis–UV and EPR), magnetic properties

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