Geometric distortions of octahedral cations and tetrahedral anions in disordered $[Cu(bpy)_3]CrO_4 \cdot 7.5H_2O$ crystal : a comparative study.

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Streszczenie

A novel copper(II) chromate complex of the formula $[Cu(bpy)_3][CrO_4] \cdot 7.5H_2O$ (**1**) (bpy = 2,2′-bipyridine) was prepared in the crystalline form and characterized by X-ray diffraction and spectroscopic methods (EPR, FIR-IR, NIR–Vis–UV). Two non-equivalent $[Cu(bpy)_3]^{2+}$ groups in the form of tetragonally elongated octahedron are built into the hydrogen-bonded network. The tetragonality parameter T is 0.9830 and 0.9876 for Cu(1) and Cu(2) centers, respectively, points to the significant Jahn–Teller (JT) distortion in the tris-bipyridine copper(II) cations. The EPR parameters g_1, g_2 and g_3 are equal to 2.168, 2.159 and 2.072, respectively, correspond to the Cu–N bond directions oscillating between long and short distances. The chromate moiety is a non-coordinated to the metal center and forms a very distorted tetrahedron with three bond lengths in the range 1.617(2)–1.629(2) Å. The O(3A) and O(3B) atoms execute reorientational motion between two equilibrium arrangements with equal probability. The related geometric distortion, Δ_r, is 0.097 Å. The Gaussian analysis of single crystal electronic spectra was based on the four d–d bands assigned for Cu(II) center to the $^2A_{1g(dx2-y2)} \rightarrow {}^2A_{2g(dz2)}$, $^2B_{1g(dxy)}$, $^2B_{2g(dxz)}$ and $^2B_{3g(dyz)}$ transitions in D_{2h} symmetry.

Słowa kluczowe

Chromate(VI) and copper(II) complexes, X-ray diffraction, EPR, IR and UV–Vis–NIR spectroscopy, Single crystal electronic spectra at 4.2 K, Gaussian analysis

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