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Structural confirmation of the 3,5-dinitrosalicylato anion coordination ability to metal ion: crystal structure, spectral and magnetic properties of the $[Cu_3\{3,5\text{-}(NO_2)_2sal^{2-}\}_2\{3,5\text{-}(NO_2)_2sal^{1-}\}_2(H_2O)_4]\cdot 4H_2O$.

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Streszczenie

Reaction of copper(II) salts with 3,5-dinitrosalicylic acid yields to the complex formation of the composition $[Cu_3\{3,5\text{-}(NO_2)_2sal^{2-}\}_2\{3,5\text{-}(NO_2)_2sal^{1-}\}_2(H_2O)_4] \cdot 4H_2O$ ($3,5\text{-}(NO_2)_2sal^{x-}$ = 3,5-dinitrosalicylate anion). The complex was characterized, by elemental microanalysis, electronic, IR and EPR spectra and magnetic susceptibility measurements. The crystal structure of the complex has been determined and refined to R = 0.0482, and wR = 0.1206 for 2980 reflections with $I > 2\sigma(I)$ (R = 0.0724, and wR = 0.1283 for all 4124 reflections. The complex crystallizes in monoclinic system, space group $P2_1/c$, a = 10.873(2), b = 14.726(3), and c = 13.167(3) Å, β = 94.11(3)°, V = 2102.8(8) Å^3, and Z = 4. Structure of the complex comprises of the centrosymmetric $[Cu_3\{3,5\text{-}(NO_2)_2sal^{2-}\}_2\{3,5\text{-}(NO_2)_2sal^{1-}\}_2(H_2O)_4]$ molecules and the water molecules which are held together by system of different types of hydrogen bonds and van der Waals interactions. The Cu(1) atom is centrosymmetrically coordinated by two 3,5-dinitrosalicylato dianions, thus forming the square planar CuO_4 chromophore. Each of the satellite Cu(2) atoms are coordinated by one oxygen atom of bridging 3,5-dinitrosalicylato dianion, two oxygen atoms of chelating 3,5-dinitrosalicylato monoanion (in the phenolato form), and by two water oxygen atoms in the square pyramidal coordination polyhedron. Variable-temperature magnetic susceptibility measurements (1.9–300 K) show occurrence of significant ferromagnetic interactions caused by *syn–anti* conformation of carboxylato bridges within the trimer (J_{12} = 4.31, J_{13} = 0 cm^{-1}). Bellow 3 K, antiferromagnetic intermolecular interaction between trimeric molecules in the crystal lattice was observed (zJ' = −0.29 cm^{-1}). The EPR spectroscopy is in agreement with the molecular structure of the complex and magnetic properties, indicates superposition spectra of copper centres (S = 1/2) with square-planar and square pyramidal coordination polyhedrons ($g_\parallel$ = 2.32, $g_\perp$ = 2.05).

Słowa kluczowe

Copper, Ion, 5-Dinitrosalicylate complex, Trimer, Crystal structure, Magnetic properties, Spectral properties

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