Syntheis, spectral and magnetical characterization of monomeric [Cu(2-NO_2bz)$_2$(nia)$_2$(H_2O)$_2$] and structural analysis of similar [Cu(RCOO)$_2$(L–N)$_2$(H_2O)$_2$]complexes.

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Streszczenie

A new complex of composition [Cu(2-NO_2 bz)$_2$ (nia)$_2$ (H_2 O)$_2$] (1) (nia=nicotinamide, 2-NO_2 bz=2-nitrobenzoate) has been prepared and its composition and stereochemistry as well as coordination mode have been determined by elemental analysis, electronic, infrared and EPR spectroscopy, magnetization measurements over the temperature range 1.8–300K, and its structure has been solved, as well. The complex structure consists of the centrosymmetric molecules with Cu(II) atom monodentately coordinated by the pair of 2-nitrobenzoato anions and by the pair of nicotinamide molecules, forming nearly tetragonal basal plane, and by a pair of water molecules that complete tetragonal–bipyramidal coordination polyhedron about the copper atom. The complex 1 exhibits magnetic moment μ_{eff} =1.86B.M. at 300K which decreases to μ_{eff} =1.83B.M. at 1.8K. The magnetic susceptibility temperature dependence obeys Curie–Weiss law with Curie constant of 0.442cm^3 Kmol^{-1} and with Weiss constant of −1.0K. EPR spectra at room temperature as well as at 77K are of axial type with $g_\perp$ =2.065 and $g_\parallel$ =2.280 and exhibit clearly, but partially resolved parallel hyperfine splitting with $A_\parallel$ =160G, that is consistent with the determined molecular structure of 1. In order to analyze the factors influencing the degree of tetragonal distortion of coordination polyhedron, the dataset of 72 structures similar to that of 1 was extracted from CCD and analyzed. A significant correlation between the average Cu–O_{ax} bond length and tetragonality parameter τ which was found as a consequence of the Jahn–Teller effect.

Słowa kluczowe

Copper, Carboxylate complexes, Crystal structure, Spectral properties, Magnetic properties, Nicotinamide