Preparation, structure, spectral and magnetic properties of copper(II) halogenonicotinates: crystal and molecular structure of tetrakis(μ-2-chloronicotinato-*O*,*O*')-diaquadicopper(II).

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Kolekcja

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Streszczenie

The characterization of the complexes $[Cu_2(2\text{-}Clnic)_4(H_2O)_2]$ (**1**), $[Cu(2,6\text{-}Cl_2nic)_2(H_2O)_2]$ (**2**) and $[Cu(5\text{-}Brnic)_2(H_2O)_2]_n$ (**3**) (where 2-Clnic = 2-chloronicotinate, 2,6-Cl_2nic = 2,6-dichloronicotinate or 5-Brnic = 5-bromonicotinate) was based on elemental analysis, IR, electronic and EPR spectra, and magnetic susceptibility. Complex **1** was also studied by X-ray analysis at 298 **1a** and 80 K **1b**. The complex **1** contains a dinuclear Cu-acetate molecular structure in which the carboxyl groups of the 2-chloronicotinate ligands act as bridges and water molecules are at apical positions. The stereochemistry about Cu atom at both temperatures is typical for square pyramidal geometry with CuO_4O chromophore. The Cu-Cu distance is 2.6513(8) and 2.6382(6) Å for **1a** and **1b**, respectively. The Cu atoms are displaced by 0.2069(9) and 0.1973(7) Å, respectively, from the plane containing four oxygen atoms bonded to the Cu atom toward the apical water molecules. Strong and weak hydrogen bonds as well as C–Cl···π interactions in the crystal structure are discussed as well. Both complexes, monomeric $[Cu(2,6\text{-}Cl_2nic)_2(H_2O)_2]$ (**2**) and polymeric $[Cu(5\text{-}Brnic)_2(H_2O)_2]_n$ (**3**), possess octahedral copper(II) stereochemistry with differing tetragonal distortions.

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