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Role of non-covalent interactions in three copper(II) 5-chloro-2-nitrobenzoate complexes with N-donor ligands: syntheses, characterization and packing analyses of trans-[Cu(β-pic)$_2$(H$_2$O)$_2$(5-chloro-2-nitrobenzoate)$_2$], trans-[Cu(γ-pic)$_2$(5-chloro-2-nitrobenzoate)$_2$] and [trans-Cu(en)$_2$(H$_2$O)$_2$](5-chloro-2-nitrobenzoate)$_2$·2H$_2$O.

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Streszczenie

Three new copper(II) complexes trans-[Cu(β-pic)2(H2O)2(5-chloro-2-nitrobenzoate)2] 1, trans-[Cu(γ-pic)2(5-chloro-2-nitrobenzoate)2], 2 and [trans-Cu(en)2(H2O)2](5-chloro-2-nitrobenzoate)2·2H2O, 3 (where β-pic = β-picoline, γ-pic = γ-picoline and en = ethylenediamine) were prepared by the addition of β-pic, γ-pic and en, respectively, to the hydrated copper(II) 5-chloro-2-nitrobenzoate, suspended in methanol-water mixture (4:1, v/v). The newly synthesized complexes have been characterized by elemental analyses, TGA, spectroscopic techniques (FT-IR, UV-Vis and EPR), conductivity measurements, magnetic susceptibility studies and single crystal X-ray structure determination. Complex 1 crystallizes in monoclinic crystal system with P21/c space group whereas the complexes 2 and 3 crystallizes in triclinic crystal system with P1^{-} space group. Single crystal X-ray structure determination revealed the presence of elongated octahedral geometry in all three complexes. Cu(II) center is covalently coordinated by two 5-chloro-2-nitrobenzoate, two β-pic moieties and two water molecules in complex 1, two bidentate 5-chloro-2-nitrobenzoate and two γ-pic moieties in complex 2. In complex 3, the copper ion is coordinated to two chelating en ligands, two water molecules; with two 5-chloro-2-nitrobenzoate as counter anions and two water molecules of crystallization. The crystal lattice in complexes 1-3 is stabilized by an intricate network of hydrogen bonding interactions (C-H...O, O-H...O in complex 1, C-H...O in complex 2 and O-H...O, N-H...O and C-H...O in 3). Besides this, π...π stacking interactions in complex 1 and C-H...π interactions in complex 2 also contribute towards stability of the crystal lattice.

Słowa kluczowe

X-ray structure, N-donor ligands, 5-chloro-2-nitrobenzoate, Non-covalent interactions

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