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Effect of the nature of second-sphere cation on the architecture of crystalline π-complexes $Ca[CuCl_2(HOCH_2C{\equiv}CCH_2OH)]_2{\cdot}4H_2O$ and $(C_7H_5N_2H_2)[CuCl_2(HOCH_2C{\equiv}CCH_2OH)]$.

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Streszczenie

In the MCl-CuCl-HOCH2C≡CCH2OH (M = Ca, C7H5N2H +2) system, the crystals of two anionic Ca[CuCl2(HOCH2C≡CCH2OH)]2-4H2O (1) and (BimH)[CuCl2(HOCH2C≡CCH2OH)] (2) (BimH+ is cation of benzimidazole-C7H5N2H +2) π-complexes are obtained and studied by single crystal X-ray diffraction Crystals of 1 are monoclinic: C2/c space group, a = 8.323(3) Å, b = 13.283(4) Å, c = 16.741(5) Å, β = 92.35(3)°, V = 1849.3(10) Å3, Z = 4; crystals of 2 are triclinic: P1 space group, a = 6.901(3) Å, b = 9.898(4)Å, c = 9.987(4) Å, α = 94.91(3)°, β = 93.91(3)°, γ = 107.59(4)°, V = 644.7(5) Å3, Z = 2. Complex 1 consists of infinite bimetallic chains [Ca(H2O)4CuCl2(HOCH2C≡CCH2OH)2]∞ forming a three-dimensional framework through (Ow)HCl and (C)O-HCl hydrogen bonds. Compound 2 is built from discrete anions [CuCl2(HOCH2C≡CCH2OH)]- paired by edge-to-edge packing in the [100] direction and large BimH+ cations with face-to-face packing. In both structures, the π-coordinated Cu(I) atom has the trigonal environment involving two Cl- anions and C≡C 2-butyne-1,4-diol bond (Cu-(C≡C) distance is 1.918(2) Å and 1.910(4) Å for 1 and 2 respectively).

Słowa kluczowe

Copper(I), π-complexes, 2-butyne-1, 4-diol, crystal structure

Adres publiczny

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