$Cu_2[Cu(H_2O)_4][(CH_2)_4(NH_3)_2][C_6H_2(COO)_4]_2 \cdot 4H_2O$ — A Three-Dimensional Coordination Polymer with Negativ Excess Charge and Channel-like Voids

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Abstract

Triclinic single crystals of $Cu_2[Cu(H_2O)_4][(CH_2)_4(NH_3)_2][C_6H_2(COO)_4]_2 \cdot 4H_2O$ have been prepared in aqueous solution at 55 °C. Space group $P1^-$ (no. 2), a = 799.73(7), b = 977.43(8), c = 1086.27(9) pm, α = 87.194(7), β = 84.679(7), γ = 74.744(6)°, V = 0.81540(12) nm^3, Z = 1. There are two unique Cu^{2+} with CN 4+1 (Cu(1)) and CN 4+2 (Cu(2)), respectively. The Cu-O distances range from 197.4(2) to 214.9(2) pm (Cu(1)) and 191.6(2) to 240.1(4) pm (Cu(2)). There is a short Cu(1)-Cu(1) contact of 267.02(6) pm. A three-dimensional coordination polymer with negative excess charge and channel-like voids extending parallel to [-110] is made up by Cu^{2+} and $[C_6H_2(COO)_4]^{4-}$. These voids accomodate $[(CH_2)_4(NH_3)_2]^{2+}$ and water molecules, which are not coordinated to Cu^{2+}. Thermoanalytical measurements in air indicated a step-wise loss of water of crystallization commencing at 63 °C, which is finished at approx. 250 °C followed by an exothermic decomposition yielding CuO. The Cu(1) pairs show anti-ferromagnetic coupling.