Structure of complexes formed in the CuX_2-Cu-*N*-allylisoquinolinium chloride system (X = Cl, Br).

Autorzy

Ya. E. Filinchuk

A. V. Pavlyuk

Zbigniew Ciunik

M. G. Mys'kiv

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The crystals of *N*-allylisoquinolinium chlorides of the compositions $[C_9H_7N(C_3H_5)]_2Cu^{II}Cl_4$ (**I**), $[C_9H_7N(C_3H_5)]Cu^{I}Cl_2 \cdot H_2O$ (**II**), and $[C_9H_7N(C_3H_5)]Cu^{I}Cl_{1.43}Br_{0.57} \cdot H_2O$ (**III**) were prepared by alternating-current electrosynthesis. X-ray diffraction analysis (using diffractometer models DARCH1 for **I**, STOE for **II**, and KUMA/CCD for **III**, MoK_α radiation) showed that the crystals of **I** are monoclinic, space group $P2_1/n$, a = 14.91(1) Å, b = 10.41(1) Å, c = 16.90(1) Å, γ = 109.73(8)°, V = 2470(8) Å^3, Z = 4. The crystals of isostructural compounds **II** and **III** are triclinic, space group $P\bar{1}$, Z = 2; crystals **II**: a = 7.2446(6) Å, b = 7.4379(6) Å, c = 12.110(1) Å, α = 80.95(1)°, β = 85.55(1)°, γ = 86.60(1)°, V = 641.8(2) Å^3; crystals **III**: a = 7.253(2) Å, b = 7.459(4) Å, c = 12.151(5) Å, α = 80.82(4)°, β = 83.73(3)°, γ = 86.81(4)°, V = 644.6(9) Å^3. The structure of **I** is composed of $Cu^{II}Cl_4^{2-}$ tetrahedra and *N*-allylisoquinolinium cations united by C–H···Cl hydrogen bonds in corrugated layers. The crystal structures of π-complexes **II** and **III** are built of $[C_9H_7(C_3H_5)]_2Cu_2{}^{I}X_4$ dimers, which form layers along the c axis due to the C–H···X hydrogen bonds. An important role in the structure formation is played by water molecules, which crosslink the organometallic layers to form a three-dimensional framework through the O–H···X contacts.

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