A-6 17:25~17:40

Crystal Structure of Copper(II) Complex of 4,11-Bis(2-pyridylmethyl)-2,5,9,12-tetramethyl-1,4,8,11-tetraazacyclotetradecane

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The complex $[Cu(L)]Cl_2 \cdot 4H_2O$ (1) (L = 4,11-bis(2-pyridylmethyl)-2,5,9,12-tetramethyl-1,4,8,11-tetraazacyclotetradecane) has been prepared and characterized by X-ray crystallography. 1 crystallizes in the monoclinic space group *C2/c*, a = 18.508(7) Å, b = 8.911(1) Å, c = 20.129(5) Å, β = 111.19(2)° , V = 3095.2(15) Å^3, Z = 4. The structure of 1 comprises a centrosymmetric cation with anions and water molecules on general sites. In complex 1, the copper atom is six-coordinate as a consequence of interaction of the secondary and tertiary amines and two nitrogen atoms of the axial pyridylmethyl groups. However, the axial Cu-N(3) (pyridylmethyl) (2.514(6) Å) is much longer than that of average Cu-N bond distance (2.054(4) Å) in the basal plane. The strong tetragonal distortion may be attributed to the well-known Jahn-Teller effect. The long contact is believed to be stabilized by hydrogen bondings composed of secondary amine, water molecules and chloride anions.