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The crystal structure of aqua-bis(6-chloropicolinato-κ²N,O)copper(II), C₁₂H₈Cl₂N₂O₅Cu

Abstract

C₁₂H₈Cl₂N₂O₅Cu, triclinic, P₁ (no. 2), a = 6.800(2) Å, b = 9.086(3) Å, c = 11.363(4) Å, α = 86.701(6)°, β = 84.830(5)°, γ = 77.353(5)°, V = 681.7(4) Å³, Z = 2, Rgt(F) = 0.0250, wRref(F²) = 0.0655, T = 296(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

To a solution of 6-chloropyridine-2-carboxylic acid (2 mmol) in anhydrous methanol (30 mL) was successively added copper acetate (1 mmol), and then maintained for 4 h at 55 °C with stirring, and then filtered at 55 °C. The filtrate was left to slowly evaporate at room temperature for 15 days, and then the precipitated green rod crystals of the title compound were filtered off. Yield: 31.5%.

Anal. Calcd. for C₁₂H₈Cl₂N₂O₅Cu: C, 36.52; H, 2.04; N, 7.10; found: C, 36.61; H, 2.03; N, 7.06.

Experimental details

A suitable crystal was selected and mounted on a Bruker APEX-II CCD. Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

In the past Cisplatin, a representative of platinum metal complexes, played an important role in clinical chemotherapy for various cancers [3–5]. Nevertheless, these drugs have severe toxicity and drug resistance, which makes it urgent to design and synthesize new antitumor drugs with potential biological activity, high efficiency and low toxicity [6–8]. In the recent study, the chemical structures of thiophene and pyridine with heterocyclic compounds have antibacterial, anticancer and anti-inflammatory effects. Pyridine ring drugs have the ability to enhance the binding of drugs to biomacromolecules and resist cancer [8].

Single crystal X-ray diffraction analysis demonstrates that the asymmetric unit of the title structure contains one copper(II) cation, two 6-chloropyridine-2-carboxylate...
ligands and one H₂O ligand. The bond distances of Cu–N are 1.9887(17) and 2.1167(17) Å, bond lengths of Cu–O are 1.9154(16) to 2.0980(16) Å, respectively, which are similar with reference [9–11]. In the title complex, the bond angles of O(3)-Cu(1)-N(1), O(5)-Cu(1)-N(2), O(3)-Cu(1)-O(1), N(1)-Cu(1)-O(1), O(5)-Cu(1)-O(1) and O(1)-Cu(1)-N(2) are 177.06(6)°, 145.02(8)°, 99.31(6)°, 80.70(6)°, 107.00(8)° and 107.53(7)°, respectively, which suggests a distorted square-pyramidal geometry [12].

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References