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The crystal structure of aqua-bis(6-chloropicolinato-κ²*N*,*O*)copper(II), $C_{12}H_8Cl_2N_2O_5Cu$

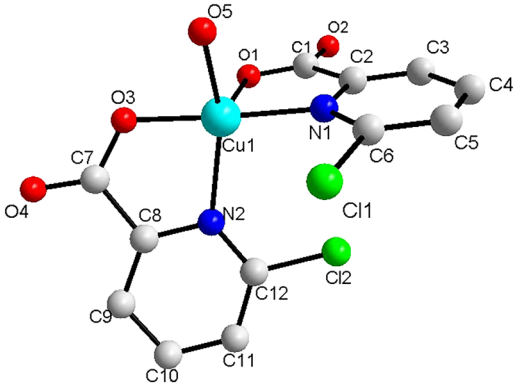

Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.20 × 0.20 × 0.20 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	2.02 mm^{-1}
Diffractometer, scan mode:	Bruker Smart APEX-II, *φ* and *ω*
θ_{max}, completeness:	27.1°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4692, 2998, 0.013
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2704
$N(param)_{refined}$:	205
Programs:	Bruker [1], SHELX [2]

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Abstract

$C_{12}H_8Cl_2N_2O_5Cu$, triclinic, $P\bar{1}$ (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) Å^3, Z = 2, $R_{gt}(F)$ = 0.0250, $wR_{ref}(F^2)$ = 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 $C_{12}H_8Cl_2N_2O_5Cu$: 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 Smart 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

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.63033 (4)	0.79121 (3)	0.65841 (2)	0.02320 (8)
Cl1	0.33740 (9)	0.64066 (7)	0.85624 (5)	0.03863 (14)
Cl2	0.89300 (9)	0.47344 (7)	0.83728 (5)	0.03834 (14)
O1	0.8697 (2)	0.89883 (18)	0.67337 (13)	0.0331 (3)
O2	1.0344 (2)	0.97638 (18)	0.81051 (14)	0.0334 (3)
O3	0.6288 (2)	0.79805 (16)	0.48969 (12)	0.0312 (3)
O4	0.6447 (3)	0.6574 (2)	0.33334 (13)	0.0406 (4)
O5	0.3755 (3)	0.9528 (2)	0.66144 (16)	0.0488 (5)
H5A	0.2761 (12)	0.9273 (13)	0.6955 (15)	0.073*
H5B	0.366 (2)	1.0096 (15)	0.6026 (9)	0.073*
N1	0.6219 (2)	0.79432 (18)	0.83367 (14)	0.0220 (3)
N2	0.7572 (2)	0.56074 (18)	0.62878 (14)	0.0219 (3)
C1	0.9011 (3)	0.9177 (2)	0.77804 (17)	0.0243 (4)
C2	0.7600 (3)	0.8614 (2)	0.87388 (17)	0.0236 (4)
C3	0.7757 (4)	0.8727 (3)	0.99272 (19)	0.0335 (5)
H3	0.8731	0.9182	1.0185	0.040*
C4	0.6434 (4)	0.8150 (3)	1.07373 (19)	0.0388 (5)
H4	0.6506	0.8220	1.1545	0.047*
C5	0.5017 (4)	0.7473 (3)	1.03286 (19)	0.0347 (5)
H5	0.4105	0.7088	1.0852	0.042*
C6	0.4981 (3)	0.7379 (2)	0.91258 (18)	0.0260 (4)
C7	0.6623 (3)	0.6715 (2)	0.43735 (17)	0.0264 (4)
C8	0.7335 (3)	0.5332 (2)	0.51564 (17)	0.0236 (4)
C9	0.7806 (3)	0.3904 (3)	0.4715 (2)	0.0314 (5)
H9	0.7644	0.3764	0.3928	0.038*
C10	0.8525 (3)	0.2682 (3)	0.5461 (2)	0.0358 (5)
H10	0.8798	0.1704	0.5194	0.043*
C11	0.8824 (3)	0.2942 (2)	0.6601 (2)	0.0337 (5)
H11	0.9329	0.2146	0.7118	0.040*
C12	0.8358 (3)	0.4417 (2)	0.69683 (18)	0.0256 (4)

ligands and one H_2O 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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