

Dichloro[cyclopropyl(2-pyridylmethylene)amino]copper(II)

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Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.034
 wR factor = 0.085
Data-to-parameter ratio = 20.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $[\text{CuCl}_2(\text{C}_9\text{H}_{10}\text{N}_2)]$, is a mononuclear copper(II) complex. The Cu^{II} ion is coordinated by two N atoms of the Schiff base ligand and by two terminal Cl anions in a distorted tetrahedral geometry. In the crystal structure, the molecules are linked through intermolecular $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds, forming chains running along the b axis.

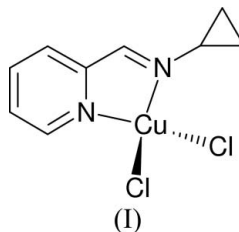
Received 6 September 2005

Accepted 9 September 2005

Online 14 September 2005

Comment

In the past few years there has been a burgeoning effort to identify the biological role of copper, primarily through techniques associated with the interface of biology/biochemistry/coordination chemistry (Collinson & Fenton, 1996; Hossain *et al.*, 1996; Tarafder *et al.*, 2002). It appears that the biological role of copper is primarily in redox reactions and as a biological catalyst, although much remains to be understood (Musie *et al.*, 2003; García-Raso *et al.*, 2003). An extensive effort has been made to prepare and characterize a variety of copper(II) coordination complexes in an attempt to model the physical and chemical behaviour of copper-containing enzymes (Reddy *et al.*, 2000). The peculiarity of copper lies in its ability to form complexes with coordination number four, five and six (Ray *et al.*, 2003; Arnold *et al.*, 2003; Raptopoulou *et al.*, 1998). As part of the investigations in this area, I report here a new mononuclear copper(II) complex, (I) (Fig. 1).



The Cu^{II} ion in (I) is four-coordinated by two N atoms of a Schiff base ligand and by two terminal Cl anions. This CuN_2Cl_2 coordination forms a distorted tetrahedral geometry, with angles subtended at the Cu atom in the range $80.81(9)$ – $115.94(3)^\circ$ (Table 1). The $\text{N1}-\text{Cu1}-\text{N2}$ bond angle [$80.81(9)^\circ$] is much smaller than the other angles around the Cu atom owing to the strain created by the five-membered chelate ring Cu1/N1/C1/C6/N2 . All the bond lengths are comparable to those of other Schiff base copper(II) complexes (Pal *et al.*, 2005; Colacio *et al.*, 1998; Shii *et al.*, 1999). The dihedral angle between the pyridine ring and the cyclopropane ring is $85.5(2)^\circ$.

In the crystal structure, the molecules are linked through intermolecular $\text{C6}-\text{H6}\cdots\text{Cl1}$ hydrogen bonds, forming chains running along the b axis (Table 2 and Fig. 2).

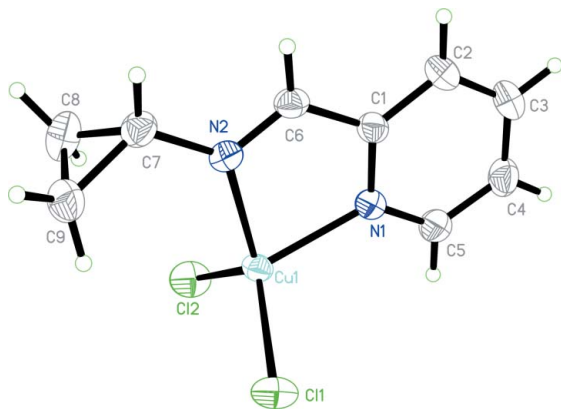


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

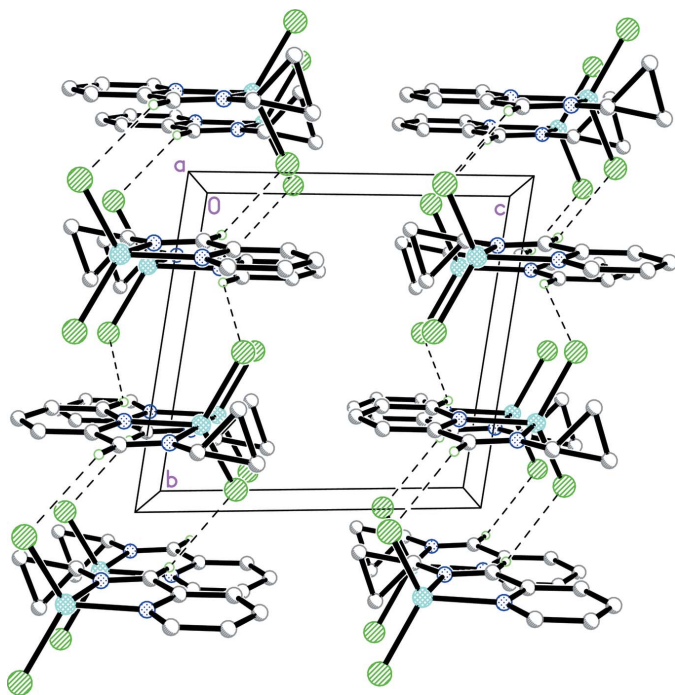


Figure 2
The crystal packing of (I). Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

Experimental

Pyridine-2-carboxaldehyde (0.1 mmol, 10.7 mg) and cyclopropylamine (0.1 mmol, 5.7 mg) were dissolved in MeOH (10 ml). The mixture was stirred for 1 h to give a yellow solution, which was added to a stirred aqueous solution (5 ml) of $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ (0.1 mmol, 17.0 mg). The mixture was stirred at room temperature for 30 min and then filtered. The filtrate was kept in air for 18 d, and blue block-shaped crystals formed. The crystals were isolated, washed three times with MeOH and dried in a vacuum desiccator containing anhydrous CaCl_2 . Yield 71.2%. Analysis calculated for $\text{C}_9\text{H}_{10}\text{Cl}_2\text{N}_2\text{Cu}$: C 38.52, H 3.59, N 9.98%; found: C 38.39, H 3.66, N 10.03%.

Crystal data

$[\text{CuCl}_2(\text{C}_9\text{H}_{10}\text{N}_2)]$
 $M_r = 280.63$
 Triclinic, $P\bar{1}$
 $a = 7.691(2) \text{ \AA}$
 $b = 8.730(2) \text{ \AA}$
 $c = 8.959(2) \text{ \AA}$
 $\alpha = 98.69(1)^\circ$
 $\beta = 99.18(1)^\circ$
 $\gamma = 91.19(1)^\circ$
 $V = 586.4(2) \text{ \AA}^3$

$Z = 2$
 $D_x = 1.589 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 5165 reflections
 $\theta = 2.3\text{--}28.4^\circ$
 $\mu = 2.28 \text{ mm}^{-1}$
 $T = 298(2) \text{ K}$
 Block, blue
 $0.32 \times 0.28 \times 0.22 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.529$, $T_{\max} = 0.634$
 6677 measured reflections

2627 independent reflections
 2542 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$
 $\theta_{\max} = 27.5^\circ$
 $h = -9 \rightarrow 9$
 $k = -11 \rightarrow 11$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.085$
 $S = 1.16$
 2627 reflections
 127 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0286P)^2 + 0.2104P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.36 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.43 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cu1—N1	2.060 (2)	Cu1—Cl2	2.2022 (9)
Cu1—N2	2.066 (2)	Cu1—Cl1	2.2114 (10)
N1—Cu1—N2	80.81 (9)	N1—Cu1—Cl1	110.24 (7)
N1—Cu1—Cl2	115.60 (7)	N2—Cu1—Cl1	114.76 (6)
N2—Cu1—Cl2	114.61 (6)	Cl2—Cu1—Cl1	115.94 (3)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
C6—H6 \cdots Cl1 ⁱ	0.93	2.81	3.573 (2)	140

Symmetry code: (i) $-x, -y, -z + 2$.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 \AA and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

The author is very grateful to Baoji College of Arts and Sciences, People's Republic of China, for funding this study.

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