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Dichlorobis[2-chloro-5-(chloromethyl)-pyridine]copper(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.053
wR factor = 0.169
Data-to-parameter ratio = 19.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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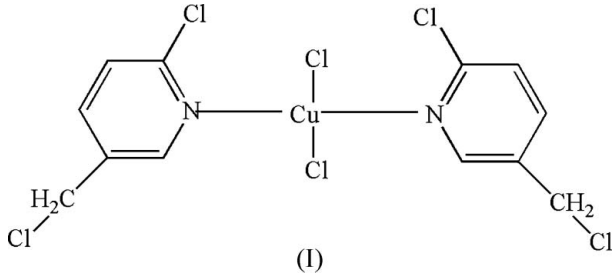
In the title compound, $[CuCl_2(C_6H_5Cl_2N)_2]$, each Cu atom has a distorted tetrahedral coordination involving two Cl^- anions and two 2-chloro-5-(chloromethyl)pyridine ligands. The molecular structure and packing are stabilized by intra- and intermolecular C—H···Cl hydrogen-bonding interactions.

Comment

The structural and magnetic properties of copper(II) complexes of the type CuL_2X_2 have been the subjects of numerous recent publications. This is particularly true for the cases where *L* is pyridine or a substituted pyridine (Swank & Willett, 1980; Marsh *et al.*, 1981; Crawford & Hatfield, 1977). Much of this work has been concerned with the correlation of the structural properties of these complexes with their magnetic properties. In order to search for new complexes of this type, we synthesized the title compound and report here its crystal structure.



(I)

The title structure contains one copper(II), two 2-chloro-5-(chloromethyl)pyridine ligands and two chloro ligands. The coordination of the copper(II) ion is best described as distorted tetrahedral. The Cu—Cl and Cu—N bond distances are in agreement with those reported recently for dichlorobis[2-(chloromethyl)pyridine]copper(II) (Zhang *et al.*, 2004). The dihedral angle formed by the pyridine rings is 18.2 (2)°. The crystal packing is stabilized by C—H···Cl intra- and intermolecular hydrogen-bond interactions (Table 2).

Experimental

The title compound was prepared by the reaction of $CuCl_2$ (0.01 mol) and 2-chloro-5-(chloromethyl)pyridine (0.02 mol) in ethanol solution (50 ml) under reflux for 4 h. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from an ethanol solution at room temperature.

Crystal data

$[CuCl_2(C_{12}H_{10}N_2)_2]$	D_x = 1.778 Mg m^{-3}
M_r = 458.47	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 25 reflections
a = 16.699 (4) Å	θ = 4–14°
b = 14.981 (5) Å	μ = 2.20 mm^{-1}
c = 15.205 (3) Å	T = 293 (2) K
β = 115.74 (3)°	Block, green
V = 3426.4 (18) Å^3	0.25 × 0.20 × 0.18 mm
Z = 8	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.044
ω scans	θ_{max} = 27.0°
Absorption correction: φ scan (North *et al.*, 1968)	$h = -21 \rightarrow 13$
T_{min} = 0.595, T_{max} = 0.673	$k = -13 \rightarrow 19$
7596 measured reflections	$l = -18 \rightarrow 18$
3689 independent reflections	3 standard reflections every 100 reflections
2778 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0948P)^2 + 8.8566P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.053	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.169	$\Delta\rho_{max}$ = 1.53 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.97 e Å^{-3}
3689 reflections	
190 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.048 (4)	Cu1—Cl4	2.2548 (14)
Cu1—N1	2.071 (4)	Cu1—Cl3	2.2965 (13)
N2—Cu1—N1	169.17 (14)	N2—Cu1—Cl3	89.53 (11)
N2—Cu1—Cl4	86.58 (11)	N1—Cu1—Cl3	94.26 (10)
N1—Cu1—Cl4	89.26 (11)	Cl4—Cu1—Cl3	175.71 (5)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···Cl3^{i}	0.93	2.70	3.390 (5)	131
C6—H6B···Cl4^{ii}	0.97	2.79	3.636 (6)	146
C9—H9A···Cl4^{iii}	0.93	2.62	3.444 (5)	149
C11—H11A···Cl5	0.93	2.83	3.140 (5)	101

Symmetry codes: (i) $-x+1, y, -z+\frac{1}{2}$; (ii) $-x+1, -y, -z+1$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

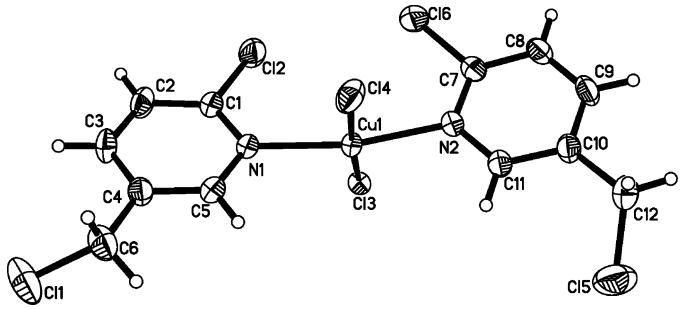


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

H atoms were positioned geometrically and allowed to ride on their attached atoms, with C—H distances = 0.93–0.97 Å and U_{iso} = 1.2U_{eq}(C). The highest peak is located 1.53 Å from atom Cl5.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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