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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.038
wR factor = 0.110
Data-to-parameter ratio = 14.9

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

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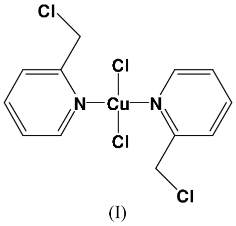
In the title compound, $[CuCl_2(C_6H_7ClN)_2]$, the Cu atom, occupying a special position on an inversion center, has a square-planar coordination formed by two Cl ligands [Cu—Cl = 2.2719 (9) Å] and two N atoms of *o*-chloromethylpyridine ligands [Cu—N = 2.008 (2) Å and Cl—Cu—N = 88.65 (8)°]. The Cl atoms of the chloromethyl groups effectively shield the axial positions of the Cu atom [Cu···Cl = 3.000 (1) Å, Cl—Cu···Cl = 90.7 (3)° and N—Cu···Cl = 74.8 (8)°].

Comment

Research into transition metal complexes has been rapidly expanding because of their fascinating structural diversity, as well as their potential applications as functional materials and enzymes (Noro *et al.*, 2000; Yaghi *et al.*, 1998). Some organic *N*-donors, such as bipyridine or related species, are often chosen for preparation of various complexes (Hagrman *et al.*, 1999). In the present paper, we report the synthesis and crystal structure of a mononuclear copper(II) complex, (I).



(I)

The crystal structure of (I) is built of discrete molecules of the complex (Fig. 1), the Cu atom occupying a special position on a crystallographic inversion center. Atom Cu1 has a typical square-planar coordination formed by two Cl ligands and two N atoms of *o*-chloromethylpyridine ligands [Cu1—Cl2 = 2.2719 (9) Å, Cu1—N1 = 2.008 (2) Å and Cl2—Cu1—N1 = 88.65 (8)°]. The Cl atoms of the chloromethyl groups occupy positions above and below the coordination plane of atom Cu1 at a distance of 3.000 (1) Å from the metal atom [the Cl1···Cu1—Cl2 and Cl1···Cu1—N1 angles are 90.74 (3) and 74.84 (8)°, respectively]. Thus, Cl1 and Cl1^i [symmetry code:

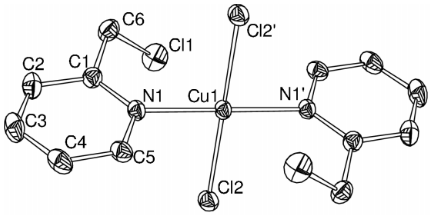


Figure 1
The structure of (I). Displacement ellipsoids are drawn at the 30% probability level. The H atoms have been omitted. [Symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}-y, -z$.]

(i) $\frac{1}{2} - x, \frac{1}{2} - y, -z$] effectively shield the axial positions in the coordination sphere of the Cu1 atom.

Experimental

To a DMF solution (10 ml) of $CuCl_2\cdot 2H_2O$ (0.085 g, 0.5 mmol), 2-chloromethylpyridine (0.128 g, 1 mmol) was added. The mixture was stirred for about 30 min and then filtered. Well shaped crystals were obtained from the mother liquor by slow evaporation at room temperature over a period of several days.

Crystal data

$[CuCl_2(C_{12}H_{12}Cl_2N_2)]$
$M_r = 389.58$
Monoclinic, $C2/c$
$a = 15.292$ (2) Å
$b = 7.7844$ (11) Å
$c = 14.306$ (2) Å
$\beta = 117.311$ (2)°
$V = 1513.2$ (4) Å^3
$Z = 4$
$D_x = 1.710$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1734 reflections
$\theta = 3.0$–25.0°
$\mu = 2.13$ mm^{-1}
$T = 293$ (2) K
Prism, blue
0.50 × 0.30 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.435$, $T_{max} = 0.626$
2252 measured reflections
1324 independent reflections
1187 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.0°$
$h = -13 \rightarrow 18$
$k = -7 \rightarrow 9$
$l = -16 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.110$
$S = 1.08$
1324 reflections
89 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0661P)^2 + 3.161P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.0122 (11)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.008 (2)	Cu1···Cl1	3.0003 (10)
Cu1—Cl2	2.2719 (9)		
N1—Cu1—Cl2	88.65 (8)	Cl2—Cu1···Cl1	90.74 (3)
N1—Cu1···Cl1	74.84 (8)		

H atoms were placed in calculated positions (C—H = 0.93—0.97 Å) and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}$(carrier atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *XPREP* in *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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