metal-organic papers

Aquadichlorobis(2-chloropyridine-κN)copper(II)

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Key indicators

In the title compound, $[CuCl_2(C_5H_4ClN)_2(H_2O)]$, the Cu^{II} atom is coordinated by one water molecule, two Cl$^-$ ions and two 2-chloropyridine molecules. The structure is built up *via* O—H···Cl hydrogen bonds and stablized by π–π stacking and Cl···Cl interactions.
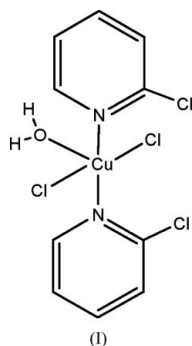
Comment

There are numerous examples of chloropyridine-coordinated complexes in the literature (Wu *et al.*, 1997; Goher *et al.*, 1997, 2003). We present here the structure of the title compound, (I), which has been synthesized for the first time.

(I)

In compound (I), the Cu^{II} atom is coordinated by N atoms from two 2-chloropyridine molecules, two Cl atoms and one water molecule (Fig. 1). The complex molecules are connected by O—H···Cl hydrogen bonds (Table 2 and Fig. 2). In addition, a π–π stacking interaction between neighbouring pyridine rings plays a subordinate role in stabilizing the structure; the centroid(x, y, z)–centroid($1 - x$, $1 - y$, $1 - z$) distance is 3.727 (4) Å.
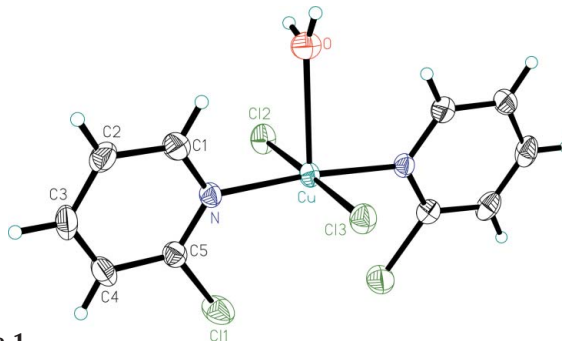
Figure 1
The molecular structure of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator $(x, -y + \frac{3}{2}, z)$.
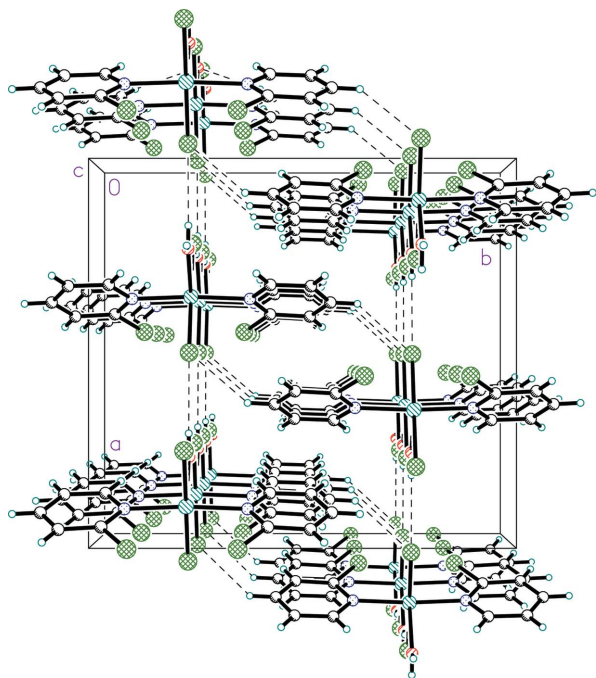
Figure 2
A view of the crystal packing of (I) along the *c* axis. Hydrogen bonds are drawn as dashed lines.

The coordination geometry around copper is square pyramidal, with a water O atom located at the apex. Compound (I) has a mirror plane passing through atoms Cu, O, Cl2 and Cl3.

It is noteworthy that there are Cl···Cl contacts (Koellner *et al.*, 1998), with Cl1···Cl3(x, y, $z + 1$) = 3.412 (4) Å and Cl1···Cl3(x, $-y + \frac{3}{2}$, $z + 1$) = 3.412 (4) Å, and these are shorter than the van der Waals distance of 3.6 Å (Gafner *et al.*, 1962; Sakurai *et al.*, 1963).

Experimental

CuCl₂·2H₂O and 2-chloropyridine, in a molar ratio of 1:2, were mixed and dissolved in sufficient ethanol by heating to 373 K, to give a clear solution. After slow cooling of the reaction mixture to room temperature, crystals of (I) were formed. These were collected and washed with distilled water.

Crystal data

[CuCl₂(C₅H₄ClN)₂(H₂O)]	Mo *Kα* radiation
$M_r = 379.55$	Cell parameters from 31
Orthorhombic, *Pnma*	reflections
$a = 14.005$ (3) Å	$\theta = 3.7–13.2°$
$b = 15.339$ (3) Å	$\mu = 2.34$ mm⁻¹
$c = 6.437$ (1) Å	$T = 296$ (2) K
$V = 1382.8$ (5) Å³	Prism, blue
$Z = 4$	$0.44 \times 0.44 \times 0.26$ mm
$D_x = 1.823$ Mg m⁻³	

Data collection

Siemens *P4* diffractometer	$R_{int} = 0.018$
ω scans	$\theta_{max} = 27.0°$
Absorption correction: ψ scan	$h = 0 \rightarrow 17$
(North *et al.*, 1968)	$k = -1 \rightarrow 19$
$T_{min} = 0.372$, $T_{max} = 0.544$	$l = 0 \rightarrow 8$
1993 measured reflections	3 standard reflections
1566 independent reflections	every 97 reflections
1117 reflections with $I > 2\sigma(I)$	intensity decay: 4.4%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0222P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.058$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.97$	$\Delta\rho_{max} = 0.30$ e Å⁻³
1566 reflections	$\Delta\rho_{min} = -0.35$ e Å⁻³
95 parameters	Extinction correction: *SHELXL97*
H atoms treated by a mixture of	(Sheldrick, 1997)
independent and constrained	Extinction coefficient: 0.0121 (5)
refinement	

Table 1
Selected geometric parameters (Å, °).

Cu—N	2.0318 (18)	Cl1—C5	1.715 (3)
Cu—Cl3	2.2720 (11)	N—C5	1.329 (3)
Cu—Cl2	2.2749 (11)	N—C1	1.339 (3)
Cu—O	2.491 (3)		
N^i—Cu—N	174.58 (12)	N—Cu—O	92.68 (6)
N—Cu—Cl3	89.29 (6)	Cl3—Cu—O	96.35 (9)
N—Cu—Cl2	90.65 (6)	Cl2—Cu—O	84.92 (9)
Cl3—Cu—Cl2	178.74 (4)		

Symmetry code: (i) x, $-y + \frac{3}{2}$, z.

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

D—H···A	D—H	H···A	D···A	D—H···A
O—H0*A*···Cl2ⁱⁱ	0.820 (10)	2.430 (12)	3.250 (3)	178 (5)
O—H0*B*···Cl3ⁱⁱⁱ	0.822 (10)	2.747 (19)	3.524 (3)	158 (5)

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

The H atoms of the water molecule were located in a difference Fourier map and refined isotropically. Other H atoms were treated as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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