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Chlorobis[2-(2-pyridyl)ethanol]copper(II) chloride

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Key indicators

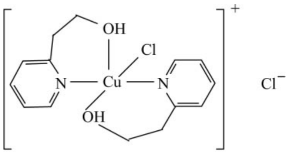
Single-crystal X-ray study
T = 133 K
Mean σ(C–C) = 0.002 Å
R factor = 0.027
wR factor = 0.069
Data-to-parameter ratio = 23.8

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

The structure of the title complex, [CuCl(pyet)$_2$]Cl [pyet is 2-(2-pyridyl)ethanol, C_7H_9NO], consists of a chloride anion and a [Cu(Cl)(pyet)$_2$]$^+$ cation. In the cation, the copper(II) ion possesses a square-pyramidal coordination geometry, with a chloro and two neutral pyet ligands. Each pyet ligand acts as an *N*,*O*-bidentate ligand and forms a six-membered chelate ring around the copper(II) ion. The H atoms of the hydroxy groups of the pyet ligands form strong hydrogen bonds with chloride ions, while the phenyl and ethylene H atoms of pyet are involved in weak interactions with both the chloro ligand and chloride ion.

Comment

This study forms part of our current research project on the synthesis and spectral, thermal and structural characterization of a series of mixed-ligand metal complexes of 2-pyridylethanol (pyet is C_7H_9NO). In this work, we report the crystal structure of a copper(II)–chloro complex, [Cu(Cl)(pyet)$_2$]Cl, of pyet.



(I)

The molecular structure of the title complex, (I), is shown in Fig. 1. Complex (I) consists of a chloride anion and a [Cu(Cl)(pyet)$_2$]$^+$ cation, in which the copper(II) ion exhibits a square-pyramidal coordination, with a chloro and two pyet ligands forming a CuN_2O_2Cl chromophore. Each pyet is neutral and acts as a bidentate (N and O) ligand, creating a six-membered chelate ring around the copper(II) ion. The basal plane of [Cu(Cl)(pyet)$_2$]$^+$ is formed by two N atoms, one

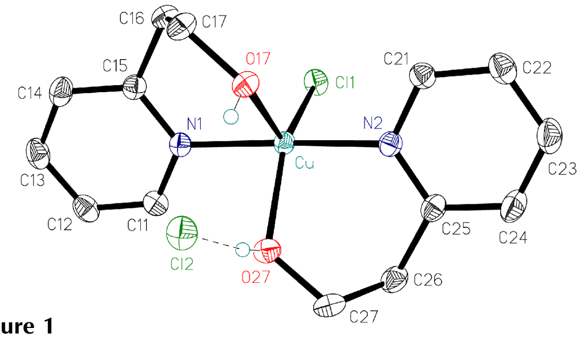


Figure 1
Molecular view of (I), showing displacement ellipsoids at the 50% probability level. Hatoms have been omitted.

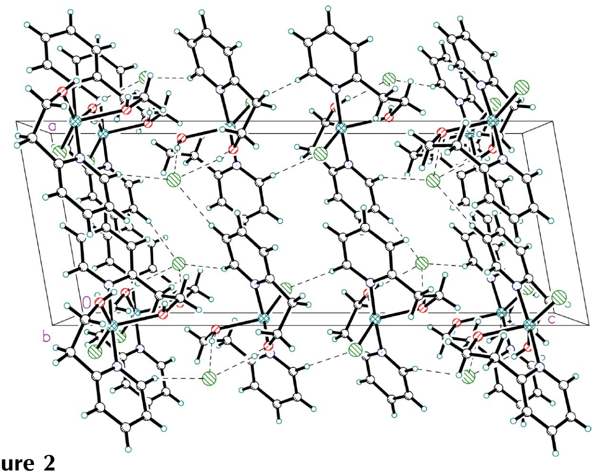


Figure 2
Packing diagram of (I).

of the hydroxy O atoms (O27) and the chloro ligand, while the apical position is occupied by the other hydroxy O atom (O17).

The Cu—N bond distances in (I) are practically identical to those found in $[Cu(H_2O)_2(pyet)_2](sac)_2$ (Yilmaz *et al.*, 2003). The Cu—O bonds are significantly longer than the Cu—N bonds. The values of the N2—Cu—N1 and O27—Cu—Cl1 bond angles indicate a significant distortion in the coordination polyhedron around the copper(II) ion. The value of the calculated structural index parameter τ (0.46) reflects the highly distorted square-pyramidal geometry [$\tau = \alpha - \beta/60$, where α and β correspond to two angles showing a tendency to linearity, and the τ values of the square-based-pyramidal and trigonal-bipyramidal extremes are 0 and 1, respectively (Addison *et al.*, 1984)]. The τ value of the title complex is very close to 0.5, which implies approximately a 50% contribution of each pyramidal extreme. However, the value of τ indicates that the copper(II) complex exhibits a greater tendency toward square-based-pyramidal geometry ($\tau > 0.5$).

The py rings are essentially planar. In the pyet ligands (C11–C17/O17/N1 and C21–C27/O27/N2), atoms C16 and C26 are almost coplanar with the mean planes of the attached py rings, but atoms O17, C17, O27 and C27 deviate from the attached py planes by 1.583 (2), 1.341 (3), 1.228 (2) and 1.334 (2) Å, respectively. The py rings are almost parallel to each other, with a dihedral angle of 165.78 (8)°. A packing diagram of (I) is shown in Fig. 2. The H atoms of the hydroxy groups of the pyet ligands form strong hydrogen bonds with the chloride ions, while the phenyl and ethylene H atoms of pyet are involved in weak interactions with both the chloro ligand and chloride ion. The molecules are held together by O—H···Cl and C—H···Cl hydrogen bonds, forming a three-dimensional network.

Experimental

Tetraaquabis(saccharinato)copper(II) dihydrate, $[Cu(H_2O)_4(sac)_2]\cdot 2H_2O$, was prepared according to the method of Haider *et al.* (1985). A butanol solution (30 ml) of $[Cu(H_2O)_4(sac)_2]\cdot 2H_2O$ (0.54 g, 1 mmol) was mixed with pyet (0.25 g, 2 mmol) and HCl (0.07 g 2 mmol) at 333 K. Single crystals suitable for X-ray diffraction were grown by slow diffusion of ether into the reaction solution at room temperature.

Crystal data

$[CuCl(C_7H_9NO)_2]\cdot Cl$
$M_r = 380.74$
Monoclinic, $P2_1/c$
$a = 8.7868 (10)$ Å
$b = 8.1911 (10)$ Å
$c = 22.718 (3)$ Å
$\beta = 100.098 (3)°$
$V = 1609.8 (3)$ Å^3
$Z = 4$

$D_x = 1.571$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7153 reflections
$\theta = 2.4$–$30.5°$
$\mu = 1.69$ mm^{-1}
$T = 133 (2)$ K
Prism, dark blue
0.44 × 0.37 × 0.29 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.522$, $T_{max} = 0.612$
28 982 measured reflections

4707 independent reflections
4445 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 30.0°$
$h = -12 \rightarrow 12$
$k = -11 \rightarrow 11$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.070$
$S = 1.11$
4707 reflections
198 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 1.0396P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—N2	1.9692 (12)	Cu—O17	2.2238 (11)
Cu—N1	1.9735 (12)	Cu—Cl1	2.2742 (4)
Cu—O27	2.0925 (11)		
N2—Cu—N1	175.30 (5)	O27—Cu—O17	88.66 (4)
N2—Cu—O27	88.73 (5)	N2—Cu—Cl1	91.67 (4)
N1—Cu—O27	87.83 (5)	N1—Cu—Cl1	92.94 (4)
N2—Cu—O17	89.24 (4)	O27—Cu—Cl1	147.77 (3)
N1—Cu—O17	87.48 (4)	O17—Cu—Cl1	123.57 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22···Cl2^{i}	0.95	2.87	3.5686 (16)	131
C21—H21···Cl2^{ii}	0.95	2.73	3.5928 (15)	152
C16—H16*A*···Cl2^{iii}	0.99	2.96	3.8767 (15)	154
C11—H11···Cl1^{iv}	0.95	2.82	3.7597 (16)	172
C26—H26*B*···Cl1^{iv}	0.99	2.94	3.6933 (16)	134
O17—H17···Cl2	0.77 (2)	2.25 (3)	3.0195 (12)	169 (2)
O27—H27···Cl2	0.76 (2)	2.22 (2)	2.9679 (12)	170 (2)

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

H atoms bonded to C atoms were included using a riding model [C—H = 0.95 or 0.99 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$], while hydroxy H atoms were refined freely [O—H = 0.76 (2) and 0.77 (2) Å].

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve

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structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

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