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catena-Poly[[[4-bromo-2-(2-pyridylmethyliminomethyl)phenolato]copper(II)]-μ-chloro]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.085
Data-to-parameter ratio = 17.9

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

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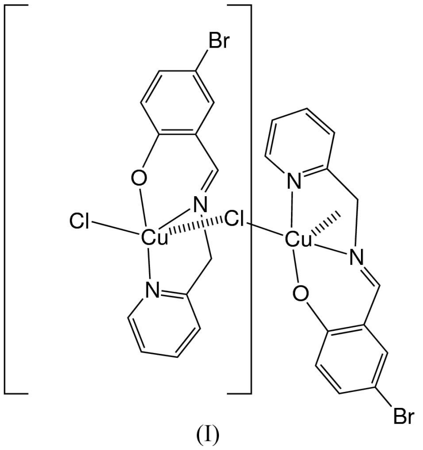
In the title compound, $[[Cu(C_{13}H_{10}BrN_2O)Cl]_n$, the Cu^{II} atom has a slightly distorted square–pyramidal coordination. The Cu atom is coordinated in the basal plane by two N atoms and one O atom of the Schiff base ligand, and by a Cl atom. The Cl atom of a symmetry-related molecule bridges the Cu atoms, so forming a slightly distorted square-pyramidal configuration at the Cu atom.

Comment

Copper compounds are present in the active sites of several important classes of metalloproteins. Studies on copper compounds are of great interest in various aspects of chemistry (Downing & Urbach, 1969; Ganeshpure *et al.*, 1996; Bosnich, 1968; Costes *et al.*, 1995). As an extension of work on the structural characterization of copper(II) complexes (Sun, 2005; Sun *et al.*, 2005), a mononuclear copper(II) complex, (I), is reported here.



(I)

Complex (I) is an infinite polynuclear copper(II) coordination polymer, as shown in Fig. 1. Selected bond distances and angles are given in Table 1. The Cu^{II} atom is four-coordinated by two N atoms and one O atom of the Schiff base ligand, and by two bridging Cl atoms, forming a slightly distorted square–pyramidal coordination configuration. The four coordinating atoms around the Cu centre in the basal plane are approximately coplanar, with an average deviation of 0.139(6) Å; the Cu atom lies 0.136 (3) Å above this plane. The Cu1—N2 bond [2.005 (3) Å] is a little longer than the corresponding values [1.985 (3) and 1.977 (4) Å] observed in two other copper(II) complexes (Sun, 2005; Sun *et al.*, 2005). The Cu1—N1 bond length [1.961 (3) Å] is also a little longer than the values [1.939 (3) and1.934(4) Å] observed in the same Schiff base complexes. The Cu1—O1 bond length [1.896 (2) Å] is

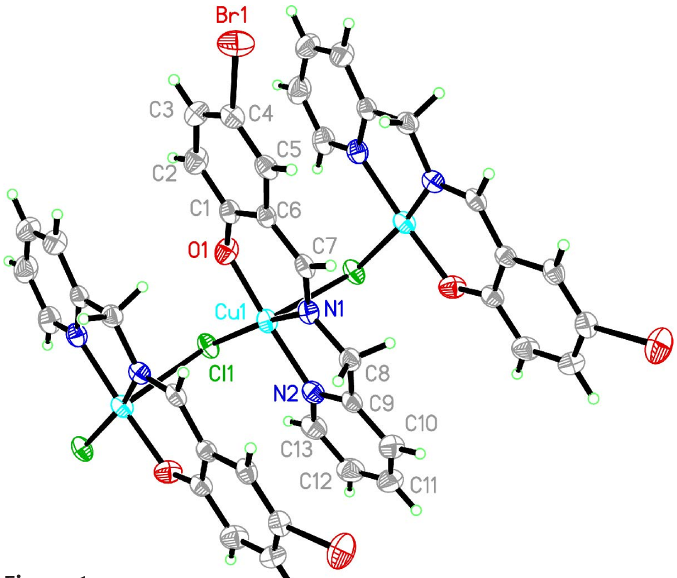


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by the symmetry code $(1 - x, y + \frac{1}{2}, -z + \frac{5}{2})$.

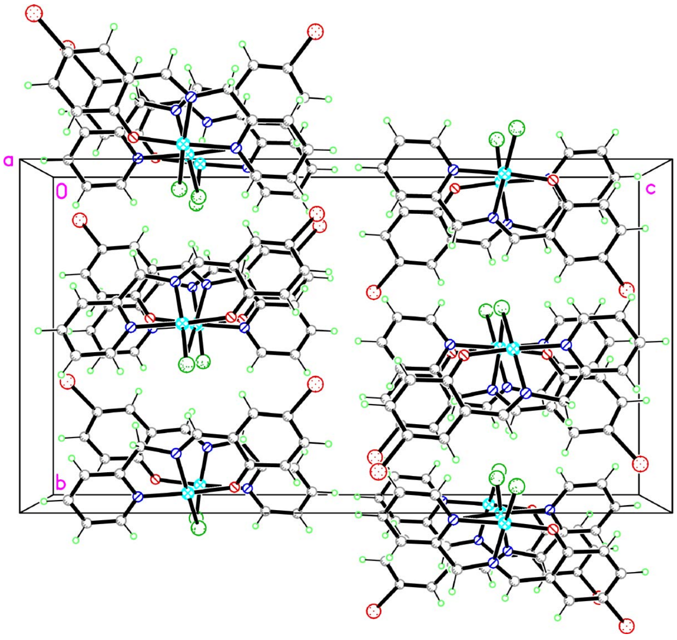


Figure 2

The crystal packing of (I), viewed along the *a* axis.

comparable to the values [1.902 (2) and 1.889 (3) Å] observed in the same complexes. The bond angles around the Cu^{II} centre show some deviations from ideal square-pyramidal geometry.

In the crystal structure, polymeric chains extend parallel to the *a* axis, as shown in Fig. 2.

Experimental

2-Aminomethylpyridine (0.1 mmol, 10.8 mg) and salicylaldehyde (0.1 mmol, 12.2 mg) were dissolved in methanol (10 ml). The mixture was stirred for 1 h to obtain a clear yellow solution. To the solution was added a methanol solution (10 ml) of $CuCl_2$ (0.1 mmol, 13.6 mg), with stirring. After keeping the resulting solution in air for 7 d, blue block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$[Cu(C_{13}H_{10}BrN_2O)Cl]$
$M_r = 389.13$
Orthorhombic, *Pbca*
$a = 7.9131$ (5) Å
$b = 13.5720$ (8) Å
$c = 25.0065$ (14) Å
$V = 2685.6$ (3) $Å^3$
$Z = 8$
$D_x = 1.925$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 4538 reflections
$\theta = 3.0–21.6°$
$\mu = 4.79$ mm^{-1}
$T = 293$ (2) K
Block, blue
0.20 × 0.08 × 0.03 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.448$, $T_{max} = 0.870$
28303 measured reflections

3073 independent reflections
1828 reflections with $I > 2\sigma(I)$
$R_{int} = 0.106$
$\theta_{max} = 27.5°$
$h = -10 \rightarrow 10$
$k = -17 \rightarrow 17$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.085$
$S = 0.85$
3073 reflections
172 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.65$ e $Å^{-3}$
$\Delta\rho_{min} = -0.34$ e $Å^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.896 (2)	Cu1—Cl1	2.272 (2)
Cu1—N1	1.961 (3)	Cu1—Cl1^i	2.819 (2)
Cu1—N2	2.005 (3)		
O1—Cu1—N1	92.88 (11)	N2—Cu1—Cl1	94.59 (9)
O1—Cu1—N2	175.46 (12)	Cl1—Cu1—Cl1^i	102.3 (2)
N1—Cu1—N2	82.65 (12)	O1—Cu1—Cl1^i	94.0 (2)
O1—Cu1—Cl1	89.93 (8)	N1—Cu1—Cl1^i	92.6 (2)
N1—Cu1—Cl1	164.66 (8)	N2—Cu1—Cl1^i	85.4 (2)

Symmetry code: (i) $1 - x, y + \frac{1}{2}, \frac{5}{2} - z$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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