metal-organic papers

[4-Bromo-2-(pyridin-2-ylmethyliminomethyl)-phenolato](methanol)copper(II) perchlorate

Yu-Xi Sun

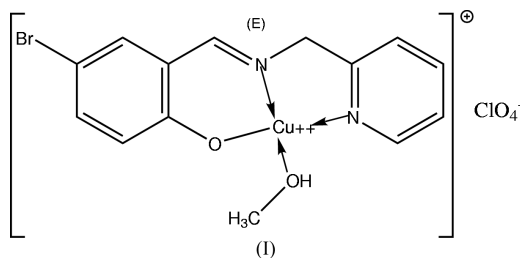Department of Chemistry, Qufu Normal University, Qufu 273165, People's Republic of China

Correspondence e-mail: yuxisun@163.com

The title compound, $[Cu(C_{13}H_{10}BrN_2O)(CH_4O)]ClO_4$, is a mononuclear copper(II) complex. The Cu^{II} atom is four-coordinated by two N atoms and one O atom of the Schiff base ligand, and another O atom of a coordinated methanol molecule, forming a slightly distorted square-planar coordination configuration. Symmetry-related cations are linked *via* a hydrogen bond, involving the coordinated methanol OH group and the coordinated O atom of the ligand, to form centrosymmetric dimers. In the crystal structure, the cations are also linked *via* the perchlorate anions [Cu1···O3 = 2.491 (7) Å] to form a polymeric structure.

## Comment

Copper compounds are present in the active sites of several important classes of metalloproteins. The study of copper compounds is 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 our work on the structural characterization of copper(II) complexes (You & Zhu, 2004; You, *et al.*, 2004) we report here the structure of the perchlorate salt, (I), of [4-bromo-2-(pyridin-2-ylmethyl-aminomethyl)phenolato](methanol)copper(II).

The molecular structure of (I) is illustrated in Fig. 1, and 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 another O atom of a coordinated methanol molecule, forming a slightly distorted square-planar coordination configuration. The four coordinating atoms around the Cu centre are approximately coplanar, giving a square-planar configuration with an average deviation of 0.042 (6) Å; the Cu atom lies 0.023 (3) Å above this plane. The Cu1—N2 bond [1.985 (3) Å; Table 1] is a little longer than the corresponding value [1.979 (2) Å] observed in another copper(II) complex (You & Zhu, 2004). The Cu1—N1 bond length [1.939 (3) Å] is also a little longer than the value [1.927 (3) Å] observed in another Schiff base complex (You *et al.*, 2004). The Cu1—O1 bond length [1.902 (2) Å] is comparable with the value [1.889 (2) Å] observed in the same
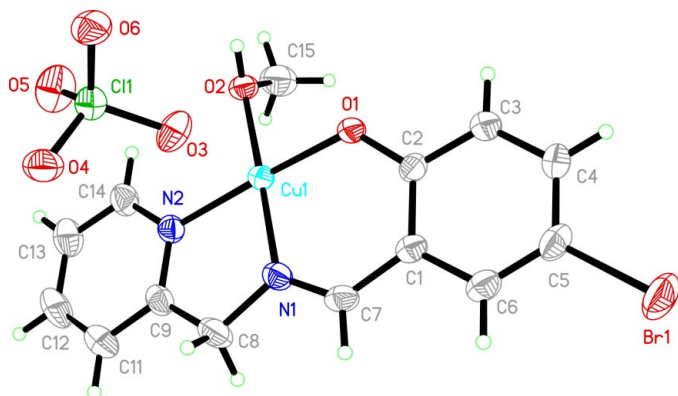
Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Only one disorder component of the anion is shown.

Schiff base complex. The bond angles around the Cu^{II} centre show some deviations from ideal square-planar geometry.

Symmetry-related cations are linked *via* a hydrogen bond, involving the coordinated methanol OH group and the coordinated O atom of the ligand, to form centrosymmetric dimers (Table 2 and Fig. 2). In the crystal structure, the cations are also linked *via* the perchlorate anions [Cu1···O3 = 2.491 (7) Å] to form a polymeric structure. The are also a number of C—H···O hydrogen bonds involving the perchlorate O atoms (more details are given in Table 2 and 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 this solution was added a methanol solution (10 ml) of Cu(ClO$_4$)$_2$·6H$_2$O (0.1 mmol, 37.1 mg), with stirring. After allowing the resulting solution to stand 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$_2$O)(CH$_4$O)]ClO$_4$
$M_r = 485.17$
Monoclinic, $P2_1/n$
$a = 7.204$ (2) Å
$b = 19.175$ (2) Å
$c = 12.716$ (2) Å
$\beta = 95.93$ (2)°
$V = 1747.2$ (6) Å^3
$Z = 4$

$D_x = 1.844$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3964 reflections
$\theta = 2.7–23.3°$
$\mu = 3.72$ mm^{-1}
$T = 295$ (2) K
Block, blue
$0.22 \times 0.21 \times 0.14$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.495$, $T_{max} = 0.624$
19 666 measured reflections

3994 independent reflections
2920 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -24 \rightarrow 24$
$l = -16 \rightarrow 16$
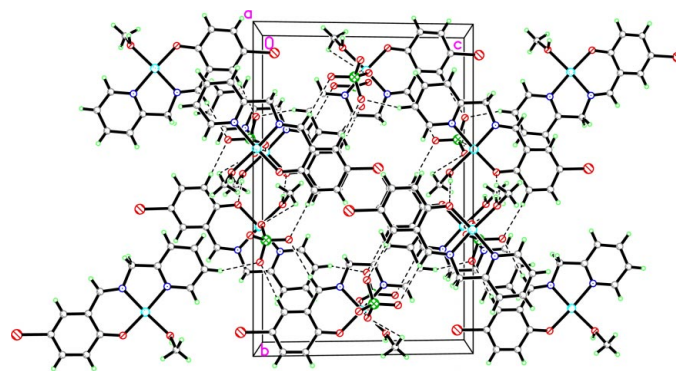
Figure 2
The crystal packing of (I), viewed along the *b* axis. Hydrogen bonds are shown as dashed lines (details are given in Table 2).

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.103$
$S = 1.03$
3994 reflections
268 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 1.3881P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.902 (2)	Cu1—N2	1.985 (3)
Cu1—O3	2.491 (7)	Cu1—O2	1.995 (2)
Cu1—N1	1.939 (3)		
O1—Cu1—N1	93.71 (11)	O1—Cu1—O2	89.72 (10)
O1—Cu1—N2	176.32 (11)	N1—Cu1—O2	174.94 (11)
N1—Cu1—N2	82.83 (12)	N2—Cu1—O2	93.82 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^i	0.84 (3)	1.87 (3)	2.686 (4)	165 (3)
C6—H6···O4^{ii}	0.93	2.31	3.223 (8)	166
C7—H7···O5^{ii}	0.93	2.54	3.432 (11)	161
C13—H13···O4^{iii}	0.93	2.36	3.256 (10)	162

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

Atom H2 was located in a difference Fourier map and was refined isotropically. All other 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 $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$. The O atoms of the perchlorate anion are disordered over two distinct sites [occupancies 0.524 (18)/0.476 (18)].

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

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