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Aqua[4-bromo-2-(pyridin-2-ylmethyliminomethyl)-phenolato]copper(II) nitrate monohydrate

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Key indicators

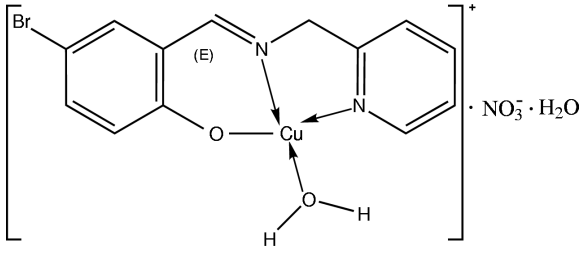
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.050
wR factor = 0.105
Data-to-parameter ratio = 15.4

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

The title compound, $[Cu(C_{13}H_{10}BrN_2O)(H_2O)](NO_3)\cdot H_2O$, is a mononuclear copper(II) complex. The Cu^{II} atom is four-coordinated by two N atoms and one O atom from the Schiff base ligand, and another O atom from a coordinated water molecule, forming a slightly distorted square-planar coordination configuration. In the crystal structure, all the O atoms in the nitrate anions and water molecules contribute to hydrogen bonds, leading to the formation of a two-dimensional network.

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).



(I)

The structure of the title complex, (I), consists of a mononuclear $[Cu(C_{13}H_{10}BrN_2O)(H_2O)]^+$ cation, a nitrate anion and an uncoordinated water molecule (Fig. 1). The Cu^{II} atom is four-coordinated by two N atoms and one O atom from the

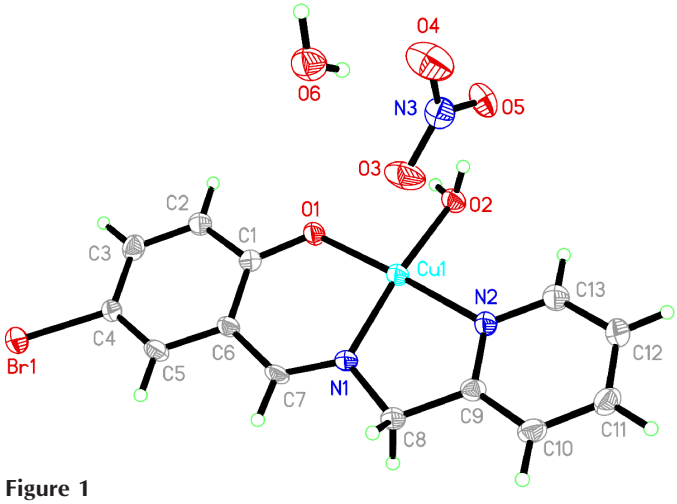


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

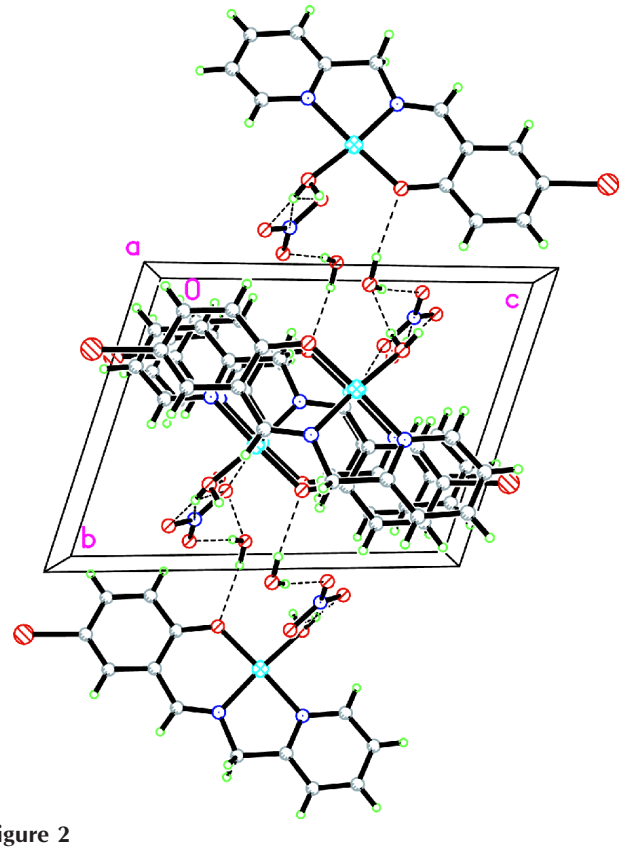


Figure 2
The crystal packing of (I), viewed along the *a* axis. The intermolecular O—H···O hydrogen bonds are shown as dashed lines.

Schiff base ligand, and another O atom from a coordinated water molecule, forming a slightly distorted square-planar coordination configuration. The four coordinating atoms around the Cu centre are approximately coplanar, with an square-planar configuration with an average deviation of 0.071 (6) Å; the Cu atom lies 0.061 (3) Å above this plane. The Cu1—N2 bond [1.977 (4) Å; Table 1] is comparable with the corresponding value [1.979 (2) Å] observed in a similar copper(II) complex (You & Zhu, 2004). The Cu1—N1 bond length [1.934 (4) Å] is 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 complex mentioned above (You *et al.*, 2004). The bond angles around the Cu^{II} centre show some deviations from ideal square-planar geometry.

In the crystal structure of (I), the molecules are linked via intermolecular O—H···O hydrogen bonds, forming a two-dimensional network (Table 2 and Fig. 2).

Experimental

2-Aminomethylpyridine (0.1 mmol, 10.8 mg) and 5-bromosalicylaldehyde (0.1 mmol, 20.1 mg) were dissolved in methanol (10 ml). The mixture was stirred for 10 min to give a clear yellow solution. To this solution was added a methanol solution (10 ml) of $Cu(NO_3)_2{\cdot}3H_2O$ (0.1 mmol, 24.2 mg), with stirring. The mixture was stirred for another 10 min to give a clear blue solution, which was allowed to evaporate slowly in the open at room temperature. After 8 d, blue block-shaped crystals were formed at the bottom of the vessel.

Crystal data

$[Cu(C_{13}H_{10}BrN_2O)(H_2O)](NO_3)\cdot H_2O$
M_r = 451.72
Triclinic, $P\overline{1}$
a = 7.838 (2) Å
b = 9.039 (2) Å
c = 11.988 (2) Å
α = 106.95 (1)°
β = 102.77 (1)°
γ = 93.04 (1)°
V = 786.0 (3) Å^3
Z = 2
D_x = 1.909 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1283 reflections
θ = 2.4–21.7°
μ = 3.97 mm^{-1}
T = 295 (2) K
Block, blue
0.17 × 0.13 × 0.12 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.530, T_{max} = 0.623
9036 measured reflections
3532 independent reflections
2255 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 27.5°
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.105
S = 0.98
3532 reflections
229 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.889 (3)	Cu1—O2	1.973 (3)
Cu1—N1	1.934 (4)	Cu1—N2	1.977 (4)
O1—Cu1—N1	93.82 (14)	O1—Cu1—N2	176.73 (14)
O1—Cu1—O2	88.90 (14)	N1—Cu1—N2	83.02 (15)
N1—Cu1—O2	171.79 (15)	O2—Cu1—N2	94.35 (15)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*B*···O6^{i}	0.84 (4)	1.84 (5)	2.658 (5)	165 (5)
O6—H6*B*···O1^{ii}	0.84 (4)	2.104 (16)	2.930 (5)	169 (5)
O2—H2*C*···O3	0.85 (5)	2.56 (5)	3.019 (5)	116 (5)
O2—H2*C*···O5	0.85 (5)	1.81 (5)	2.650 (5)	170 (5)
O6—H6*A*···O4	0.85 (5)	1.96 (5)	2.776 (6)	165 (6)

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y, -z+1$.

The H atoms of the water molecules were located in a difference Fourier map and refined isotropically, with U_{iso}(H) values fixed at 0.08 Å^2, and with O—H and H···H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 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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