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Aqua[2-(pyridin-2-ylmethyliminomethyl)phenolato-$\kappa^3 N,N',O$]copper(II) nitrate monohydrate

Zhong-Lu You,[a,b] Bo Chen,[a] Hai-Liang Zhu[a,b]* and Wei-Sheng Liu[b]

[a]Department of Chemistry, Fuyang Normal College, Fuyang, Anhui 236041, People's Republic of China, and [b]Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China

Correspondence e-mail:
hailiang_zhu@163.com

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Key indicators

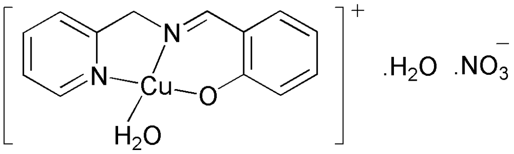
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.124
Data-to-parameter ratio = 13.8

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

The title compound, $[Cu(C_{13}H_{11}N_2O)(H_2O)](NO_3)\cdot H_2O$, is a mononuclear copper(II) compound. The Cu atom is coordinated by two N atoms and one O atom from the Schiff base ligand, and another O atom from a water molecule. The four atoms around the metal constitute a slightly distorted square-planar geometry. All O atoms in the nitrate anions and all amine N atoms in the 2-aminomethylpyridine ligands contribute to hydrogen bonds, leading to the formation of sheets parallel to the *ab* plane.

Comment

Recently, we have reported a few Schiff base complexes (You, Lin *et al.*, 2003; You, Qu *et al.*, 2003; You, Xiong *et al.*, 2004; You, Zhu & Liu, 2004). As an extension of our work on the structural characterization of Schiff base complexes, the title mononuclear copper(II) complex, (I), is reported here.



(I)

The structure of compound (I) (Fig. 1) consists of a mononuclear $[Cu(C_{13}H_{11}N_2O)(H_2O)]^+$ cation, a nitrate anion and an uncoordinated water molecule. The Cu atom is in a square-planar geometry and is four-coordinated by one O and two N atoms from the Schiff base ligand, and one O atom from the coordinated water molecule. The four coordinating atoms

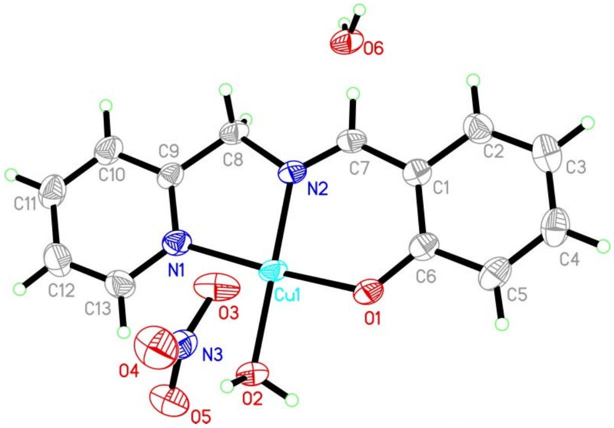


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

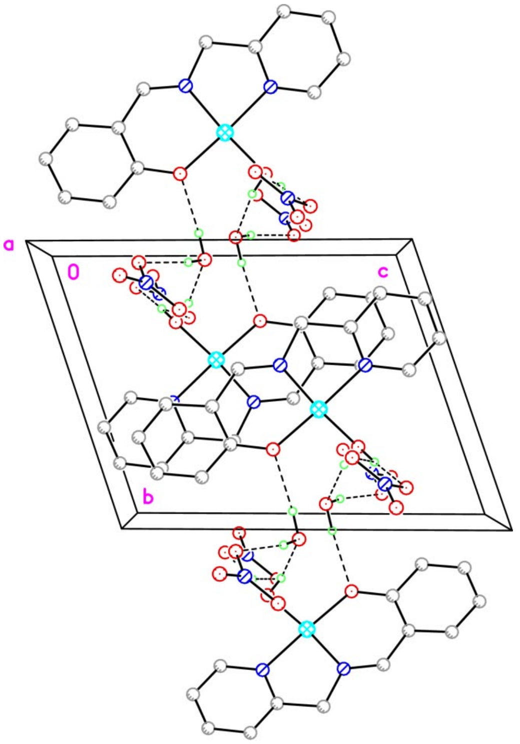


Figure 2
The crystal packing of (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

around Cu are approximately coplanar, giving a square-planar geometry with an average deviation of 0.091 (4) Å, with the Cu atom 0.064 (3) Å above this plane.

The C7—N2 bond distance of 1.282 (4) Å conforms to the value for a double bond, while the C8—N2 bond distance of 1.469 (4) Å conforms to the value for a single bond. The Cu1—O1 bond length of 1.889 (2) Å (Table 1) is a little shorter than the value of 1.914 (2) Å observed in another Schiff base complex (Langer *et al.*, 2003). The Cu1—N2 bond distance of 1.927 (3) Å is also a little shorter than the value of 1.956 (2) Å observed in the same complex. The Cu1—N1 and Cu1—O2 distances are also comparable with the values found in most copper(II) complexes (Butcher *et al.*, 2003). The bond angles around the Cu^{II} centre show some deviations from ideal square-planar geometry.

All O atoms in the nitrate anions and all amine N atoms in the 2-aminomethylpyridine ligands contribute to hydrogen bonds, leading to the formation of sheets parallel to the *ab* plane (Table 2 and Fig. 2).

Experimental

All chemicals used (reagent grade) were commercially available. Elemental analyses for C, H and N were performed on a Perkin–Elmer 240 C elemental analyser. 2-Aminomethylpyridine (0.1 mmol, 10.8 mg) and Cu(NO$_3$)·3H$_2$O (0.1 mmol, 24.2 mg) were dissolved in methanol (10 ml). The mixture was stirred for 1 h to give a clear blue solution, which was allowed to evaporate slowly in the open at room temperature. After 5 d, blue block crystals of (I) were formed at the bottom of the vessel. These crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using anhydrous CaCl$_2$ (yield 81.3%). Analysis found: C 41.9, H 4.1, N 11.3%; calculated for $C_{13}H_{15}N_3O_6Cu$: C 41.7, H 4.2, N 11.1%.

Crystal data

[Cu(C$_{13}$H$_{11}$N$_2$O)(H$_2$O)](NO$_3$)·H$_2$O
M_r = 372.82
Triclinic, $P\overline{1}$
a = 7.777 (2) Å
b = 8.993 (2) Å
c = 11.389 (2) Å
α = 71.25 (3)°
β = 86.18 (3)°
γ = 86.88 (3)°
V = 752.2 (3) Å^3
Z = 2
D_x = 1.646 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3171 reflections
θ = 2.4–26.8°
μ = 1.49 mm^{-1}
T = 293 (2) K
Block, blue
0.27 × 0.23 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
T_{min} = 0.690, T_{max} = 0.808
5940 measured reflections
3044 independent reflections
2816 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 26.5°
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.124$
S = 1.18
3044 reflections
220 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.1843P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.889 (2)	Cu1—O2	1.977 (2)
Cu1—N2	1.927 (3)	Cu1—N1	1.993 (3)
O1—Cu1—N2	93.93 (11)	O1—Cu1—N1	176.23 (10)
O1—Cu1—O2	89.19 (11)	N2—Cu1—N1	82.80 (11)
N2—Cu1—O2	170.39 (10)	O2—Cu1—N1	94.35 (11)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O5	0.897 (10)	1.787 (11)	2.680 (4)	173 (4)
O2—H2A···N3	0.897 (10)	2.47 (3)	3.248 (4)	146 (4)
O2—H2*A*···O3	0.897 (10)	2.51 (4)	3.024 (4)	117 (3)
O6—H6*B*···O4^{i}	0.896 (10)	1.951 (16)	2.825 (4)	165 (4)
O2—H2*B*···O6^{ii}	0.892 (10)	1.784 (14)	2.665 (4)	169 (4)
O6—H6*A*···O1^{iii}	0.900 (10)	2.022 (12)	2.917 (3)	173 (3)

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

Atoms H2*A*, H2*B*, H6*A* and H6*B* were located in a difference Fourier map and refined isotropically, with U_{iso}(H) values fixed at 0.08 Å^2. All remaining 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* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* and *SHELXTL* (Sheldrick, 1997*a*); program(s) used to solve structure: *SHELXS*97 (Sheldrick,

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1997*b*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Butcher, R. J., Mockler, G. M. & McKern, O. (2003). *Acta Cryst.* E**59**, m1104–m1106.

Langer, V., Scholtzová, E., Gyepesová, D., Kohútová, M. & Valent, A. (2003). *Acta Cryst.* E**59**, m1181–m1183.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*a*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1997*b*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

You, Z.-L., Lin, Y.-S., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2003). *Acta Cryst.* E**59**, m1025–m1027.

You, Z.-L., Qu, Y., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2003). *Acta Cryst.* E**59**, m1038–m1040.

You, Z.-L., Xiong, Z.-D., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, m79–m81.

You, Z.-L., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst.* E**60**, m560–m562.

m886 You *et al.* • $[Cu(C_{13}H_{11}N_2O)(H_2O)](NO_3)\cdot H_2O$ *Acta Cryst.* (2004). E**60**, m884–m886