Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Aqua{2-[2-(2-hydroxyethylamino)ethyliminomethyl]-4-nitrophenolato}copper(II) perchlorate

Zhong-Lu You

Department of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China

Correspondence e-mail:
youzhonglu@yahoo.com.cn

In the title compound, $[Cu(C_{11}H_{14}N_3O_4)(H_2O)]ClO_4$, the Cu^{II} ion is five-coordinated in a square-pyramidal configuration, with one imine N, one amine N, one phenolate O, and one hydroxyl O atom of the Schiff base defining the basal plane, and the O atom of a coordinated water molecule occupying the apical position. In the crystal structure, the molecules are linked through intermolecular O—H⋯O and N—H⋯O hydrogen bonds, forming chains running along the *b* axis.

Received 17 April 2006
Accepted 2 May 2006

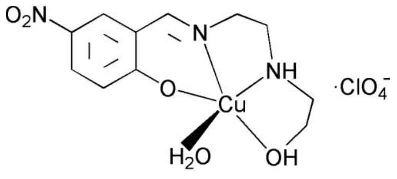
Key indicators

Single-crystal X-ray study
T = 298 K
Mean *σ*(C–C) = 0.010 Å
Disorder in solvent or counterion
R factor = 0.078
wR factor = 0.202
Data-to-parameter ratio = 12.1

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

Comment

The Schiff base ligand, 2-[2-(2-hydroxyethylamino)ethyliminomethyl]phenol (HEP), is a versatile tetradentate ligand, which forms stable complexes with a large number of transition metal ions (Zhu *et al.*, 2003; Yang *et al.*, 2004). However, the complexes related to the HEP derivative, 2-{[2-(2-hydroxyethylamino)ethyliminomethyl]-4-nitrophenol, have seldom been reported. We have focused our attention on the assembly of transition metal ions with flexible ligands, since they can adopt diverse coordination modes according to the geometric needs of the metal ions (You, 2005*a*,*b*). The author reports here a new copper(II) compound, (I).



(I)

The title compound is a mononuclear copper(II) complex (Fig. 1). The complex consists of a $[Cu(C_{11}H_{14}N_3O_4)(H_2O)]^+$ cation and a disordered perchlorate anion. The Cu^{II} atom is five-coordinated in a square-pyramidal configuration, with one imine N, one amine N, one phenolate O, and one hydroxyl O atom of the Schiff base defining the basal plane, and the O atom of a coordinated water molecule occupying the apical position. The Cu^{II} centre is displaced out of the basal plane by 0.179 (5) Å in the direction of O5. The Cu—O and Cu—N bond lengths (Table 1) are comparable to the corresponding values observed in other Schiff base copper(II) complexes (You *et al.*, 2006; You, 2006*a*,*b*; MacLachlan *et al.*, 1996; Colacio *et al.*, 2000; Mukherjee *et al.*, 2003).

In the crystal structure, the molecules are linked through intermolecular O—H⋯O and N—H⋯O hydrogen bonds (Table 2), forming chains running along the *b* axis (Fig. 2).

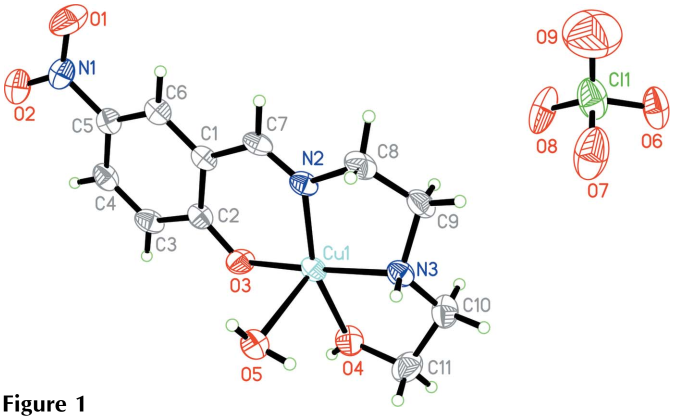


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Only one component of the disordered anion is shown.

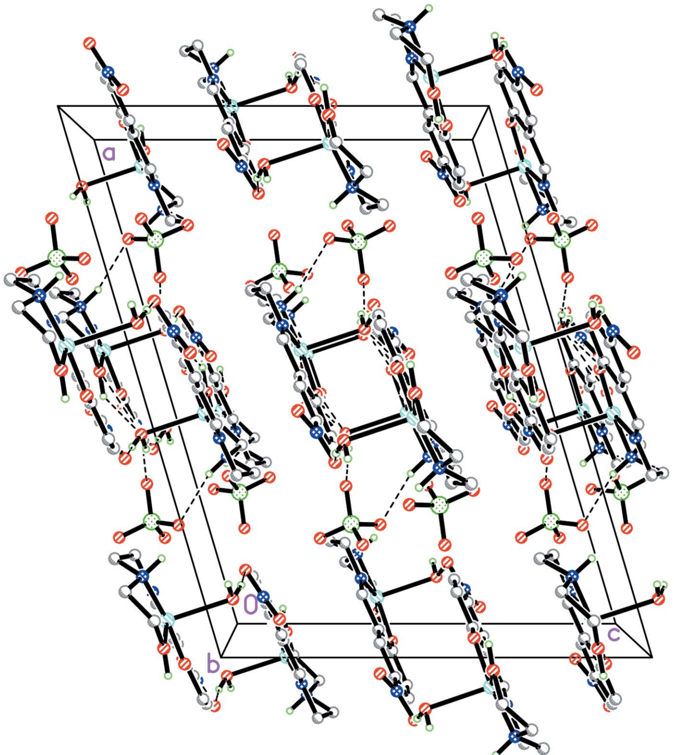


Figure 2
The crystal packing of (I), viewed along the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines. Only one component of the disordered anion is shown.

Experimental

All reagents were of commercially available grade and were used without further purification. 5-Nitrosalicylaldehyde (0.1 mmol, 16.5 mg) and 2-hydroxylaminoethylamine (0.1 mmol, 10.4 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added an aqueous solution of $Cu(ClO_4)_2 \cdot 7H_2O$ (0.1 mmol, 38.9 mg), with stirring. The mixture was stirred for another 10 min at room temperature. After keeping the filtrate in air for 2 d, blue block-shaped crystals were formed. Analysis found: C 30.33, H 3.86, N 9.83%; calculated for $C_{11}H_{16}ClCuN_3O_9$: C 30.49, H 3.72, N 9.70%.

Crystal data

$[Cu(C_{11}H_{14}N_3O_4)(H_2O)]ClO_4$
$M_r = 433.26$
Monoclinic, $C2/c$
$a = 19.552\ (2)$ Å
$b = 11.859\ (1)$ Å
$c = 14.658\ (2)$ Å
$\beta = 106.488\ (1)^\circ$
$V = 3259.0\ (6)$ Å^3
$Z = 8$
$D_x = 1.766$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.56$ mm^{-1}
$T = 298\ (2)$ K
Block, blue
$0.29 \times 0.21 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.661$, $T_{\max} = 0.800$
12264 measured reflections
3193 independent reflections
2722 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.034$
$\theta_{\max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.078$
$wR(F^2) = 0.202$
$S = 1.16$
3193 reflections
263 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0862P)^2 + 19.9923P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.07$ e Å^{-3}
$\Delta\rho_{\min} = -0.67$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.889 (5)	Cu1—N3	1.991 (5)
Cu1—N2	1.919 (5)	Cu1—O5	2.403 (5)
Cu1—O4	1.989 (5)		
O3—Cu1—N2	95.1 (2)	O4—Cu1—N3	83.3 (2)
O3—Cu1—O4	94.9 (2)	O3—Cu1—O5	90.9 (2)
N2—Cu1—O4	161.3 (2)	N2—Cu1—O5	102.8 (2)
O3—Cu1—N3	174.0 (2)	O4—Cu1—O5	92.8 (2)
N2—Cu1—N3	85.1 (2)	N3—Cu1—O5	94.8 (2)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O4—H4$A\cdots$O5$^{\rm i}$	0.93	1.98	2.795 (7)	145
N3—H3$A\cdots$O6$'^{\rm ii}$	0.91	2.04	2.854 (19)	148
N3—H3$A\cdots$O6$^{\rm ii}$	0.91	2.16	3.047 (10)	164
O5—H5$A\cdots$O8$^{\rm ii}$	0.84	1.98	2.811 (14)	169
O5—H5$A\cdots$O9$'^{\rm ii}$	0.84	2.39	3.01 (2)	131
O5—H5$B\cdots$O2$^{\rm iii}$	0.84	2.27	3.029 (8)	152
O5—H5$B\cdots$O1$^{\rm iii}$	0.84	2.58	3.055 (8)	117

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

The O atoms of the perchlorate anion are disordered over two distinct sets of sites with occupancies of 0.529 (13) and 0.471 (13). The Cl—O distances in both disordered components were restrained to 1.41 (1) Å, and the O$\cdots$O distances were restrained to be equal. The $U_{\rm ij}$ components of atoms O7, O9 and O6$'$ were restrained to approximately isotropic behaviour. Water H atoms were located in a difference map and were allowed to ride on the attached O atom, with O—H = 0.84 Åand $U_{\rm iso} = 1.5U_{\rm eq}$(O). All other H atoms were placed in calculated positions (O—H = 0.93 Å, N—H = 0.91 Å and C—H = 0.93–0.97 Å), and were constrained to ride on their parent atoms with $U_{\rm iso}$(H) set at $1.2U_{\rm eq}$(C,N) or $1.5U_{\rm eq}$(O). The highest peak in the difference map is 0.89 Å from O7$'$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); 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*.

The author acknowledges Liaoning Normal University for funding this study.

References

Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.

Colacio, E., Ghazi, M., Kivekäs, R. & Moreno, J. M. (2000). *Inorg. Chem.* **39**, 2882–2890.

MacLachlan, M. J., Park, M. K. & Thompson, L. K. (1996). *Inorg. Chem.* **35**, 5492–5499.

Mukherjee, A., Rudra, I., Naik, S. G., Ramasesha, S., Nethaji, M. & Chakravarty, A. R. (2003). *Inorg. Chem.* **42**, 5660–5668.

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

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Yang, S., Liu, Q.-X., Zeng, W.-J., Zou, Y., Wang, Z.-G. & Zhu, H.-L. (2004). *Z. Kristallogr. New Cryst. Struct.* **219**, 155–156.

You, Z.-L. (2005*a*). *Acta Cryst.* C**61**, m359–m360.

You, Z.-L. (2005*b*). *Acta Cryst.* C**61**, m532–m534.

You, Z.-L. (2006*a*). *Acta Cryst.* E**62**, m45–m46.

You, Z.-L. (2006*b*). *Acta Cryst.* E**62**, m47–m48.

You, Z.-L., Wang, J. & Han, X. (2006). *Acta Cryst.* E**62**, m860–m861.

Zhu, H.-L., Lin, Y.-S., Meng, F.-J., Zou, Y. & Wang, D.-Q. (2003). *Acta Cryst.* E**59**, m878–m879.