

Zhong-Lu You,^{a,b} Zhong-Duo Xiong^b and Hai-Liang Zhu^{a,b*}^aDepartment of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, and ^bDepartment of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of ChinaCorrespondence e-mail:
hailiang_zhu@163.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.010 \text{ \AA}$
Disorder in solvent or counterion
R factor = 0.073
wR factor = 0.240
Data-to-parameter ratio = 14.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Bis{2-[3-(diethylamino)propyliminomethyl]-phenolato}copper(II) diperchlorate

In the title centrosymmetric mononuclear copper(II) compound, $[\text{Cu}(\text{C}_{14}\text{H}_{22}\text{N}_2\text{O})_2](\text{ClO}_4)_2$, the Cu^{II} atom is coordinated by two N atoms and two O atoms from two Schiff base ligands. The coordination geometry is slightly distorted square-planar. The disordered perchlorate anions are hydrogen bonded to the cation *via* $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

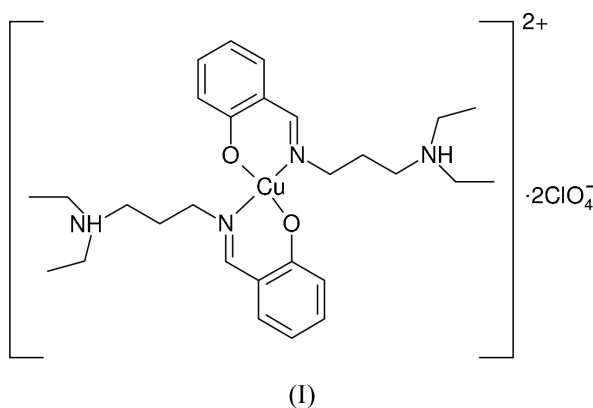
Received 1 July 2004

Accepted 7 July 2004

Online 17 July 2004

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, a mononuclear copper(II) complex, (I), is reported here.



The structure of the title compound, (I) (Fig. 1), consists of a mononuclear $[\text{Cu}(\text{C}_{14}\text{H}_{22}\text{N}_2\text{O})_2]^{2+}$ cation and two perchlorate anions. The Cu atom, on an inversion center, is in a slightly distorted square-planar geometry and is four-coordinated by two N atoms and two O atoms from two Schiff base ligands. The two *trans* angles at the copper(II) center are exactly 180° , by virtue of the crystallographic symmetry (Table 1), and the other angles are close to 90° , *viz.* $88.29(16)$ and $91.71(16)^\circ$, indicating a slight deviation from perfect square-planar geometry. The Cu1–O1 bond length [$1.888(4) \text{ \AA}$] is comparable to that observed in another Schiff base complex [$1.889(2) \text{ \AA}$; You, Chen *et al.*, 2004]. The Cu1–N1 bond distance [$2.002(4) \text{ \AA}$] is slightly longer than the value [$1.927(3) \text{ \AA}$] observed in the same previously reported complex.

In the crystal structure of (I), the perchlorate anions are hydrogen bonded to the Cu^{II} cation through $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds [$\text{H}2\cdots\text{O}2^{\text{i}} = 1.97(6) \text{ \AA}$, $\text{N}2\cdots\text{O}2^{\text{i}} = 2.959(12) \text{ \AA}$ and $\text{N}2-\text{H}2\cdots\text{O}2^{\text{i}} = 175(5)^\circ$; symmetry code: (i) $1-x, -y, 1-z$; Fig. 2].

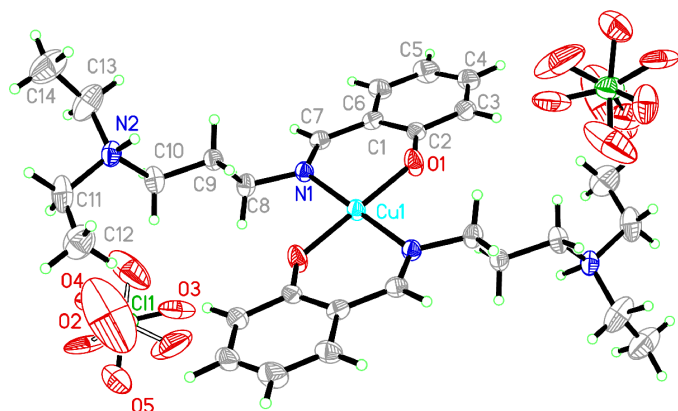


Figure 1

A view 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. Both components of the disordered perchlorate anions are shown. The unlabeled atoms are related by the symmetry operation $(1-x, -y, 1-z)$.

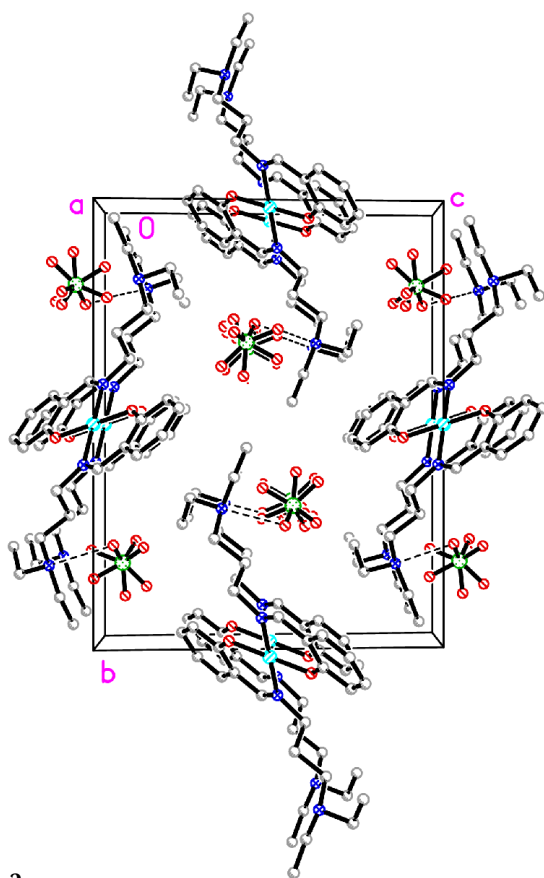


Figure 2

The crystal packing of (I), viewed along the a axis. All H atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

Experimental

N,N-Diethylpropane-1,3-diamine and salicylaldehyde were available commercially and were used without further purification. *N,N*-Diethylpropane-1,3-diamine (0.2 mmol, 26.5 mg) and salicylaldehyde (0.2 mmol, 22.4 mg) were dissolved in methanol (20 ml). The mixture was stirred for 1 h to obtain a clear yellow solution of *L* (0.2 mmol),

where *L* is 2-[(3-(diethylamino)propyl)iminomethyl]phenol. To the solution of *L* was added a solution of $\text{Cu}(\text{ClO}_4)_2 \cdot 7\text{H}_2\text{O}$ (0.1 mmol, 38.9 mg) in methanol (10 ml), with stirring. After keeping the resulting solution in air for 15 d, blue block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvents. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using anhydrous CaCl_2 (yield 82.1%). Analysis found: C 45.8, H 6.2, N 7.8%; calculated for $\text{C}_{28}\text{H}_{44}\text{Cl}_2\text{CuN}_4\text{O}_{10}$: C 46.0, H 6.1, N 7.7%.

Crystal data

$[\text{Cu}(\text{C}_{14}\text{H}_{22}\text{N}_2\text{O})_2](\text{ClO}_4)_2$
 $M_r = 731.11$
 Monoclinic, $P2_1/n$
 $a = 7.120$ (2) Å
 $b = 17.501$ (4) Å
 $c = 13.730$ (3) Å
 $\beta = 96.05$ (2)°
 $V = 1701.3$ (7) Å³
 $Z = 2$

$D_x = 1.427$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1282 reflections
 $\theta = 2.3$ – 18.4 °
 $\mu = 0.86$ mm⁻¹
 $T = 293$ (2) K
 Block, blue
 $0.32 \times 0.28 \times 0.21$ mm

Data collection

Siemens SMART CCD diffractometer
 ω scans
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.771$, $T_{\max} = 0.841$
 9156 measured reflections

3479 independent reflections
 1954 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.048$
 $\theta_{\max} = 26.5$ °
 $h = -7 \rightarrow 8$
 $k = -21 \rightarrow 21$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.074$
 $wR(F^2) = 0.240$
 $S = 1.02$
 3479 reflections
 245 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.1342P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.55$ e Å⁻³
 $\Delta\rho_{\min} = -0.34$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.888 (4)	Cu1—N1	2.002 (4)
O1—Cu1—O1 ⁱ	180	O1—Cu1—N1	91.71 (16)
O1—Cu1—N1 ⁱ	88.29 (16)	N1 ⁱ —Cu1—N1	180

Symmetry code: (i) $1-x, -y, 1-z$.

The H atom bonded to N2 was refined independently with an isotropic displacement parameter, giving an N—H distance of 0.99 (6) Å. All remaining H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C})$ for methyl atoms. The O atoms of the unique perchlorate anion are disordered over two distinct sites with a ratio of occupancies of 0.692 (3):0.308 (3).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

The authors thank the Education Office of Anhui Province, People's Republic of China, for research grant No. 2004kj300zd.

References

- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997a). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- You, Z.-L., Chen, B., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst.* **E60**, m884–m886.
- You, Z.-L., Lin, Y.-S., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2003). *Acta Cryst.* **E59**, m1025–m1027.
- You, Z.-L., Qu, Y., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2003). *Acta Cryst.* **E59**, m1038–m1040.
- You, Z.-L., Xiong, Z.-D., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2004). *Acta Cryst.* **E60**, m79–m81.
- You, Z.-L., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst.* **E60**, m560–m562.