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Acetato{2-[2-(diethylamino)ethyliminomethyl]-4-nitrophenolato}copper(II)

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In the title mononuclear copper(II) complex, $[Cu(C_{13}H_{18}N_3O_3)(C_2H_3O_2)]$, the Cu^{II} ion is four-coordinated by one Schiff base ligand and one acetate anion in a slightly distorted square-planar geometry.

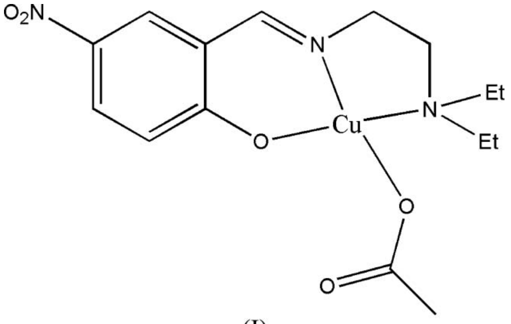
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.091
Data-to-parameter ratio = 17.4

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

Comment

Recently, we have reported the crystal structures of a few Schiff base–metal complexes (You *et al.*, 2006*a*,*b*; You, Han *et al.*, 2006). As an extension of this work, the crystal structure of the title mononuclear copper(II) complex, (I) (Fig. 1), is reported here.



(I)

The Cu^{II} ion in (I) is four-coordinated by the *NNO* donor set of the Schiff base ligand, and by one O atom of the acetate anion in a slightly distorted square-planar geometry. The Cu—O and Cu—N bond lengths (Table 1) are comparable to those in other Schiff base–copper(II) complexes (You, 2006; You & Zhu, 2006; You *et al.*, 2006*a*,*b*; You, Han *et al.*, 2006; You, Jiao *et al.*, 2006). The two *trans* angles at the metal centre are 171.54 (6) and 166.21 (7)°; all other angles around Cu1 are close to 90°, ranging from 84.63 (7) to 93.55 (6)°, indicating a slightly distorted square-planar geometry for Cu1.

In the crystal structure, molecules are linked through intermolecular C—H···O hydrogen bonds (Table 2), forming a ribbon along the *b* axis.

Experimental

All reagents were of commercially available grade and were used without further purification. 5-Nitro-2-hydroxybenzaldehyde (0.1 mmol, 16.5 mg) and *N*,*N*-diethylethane-1,2-diamine (0.1 mmol, 11.6 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min, giving a clear orange solution. To this solution was added an aqueous solution (1 ml) of $Cu(CH_3COO)\cdot H_2O$ (0.1 mmol, 20.0 mg) with stirring. The mixture was stirred for a furher 10 min at room temperature. After leaving the filtrate to stand in air for 6 d, blue block-shaped crystals of (I) were formed.

Crystal data

$[Cu(C_{13}H_{18}N_3O_3)(C_2H_3O_2)]$
$M_r = 386.89$
Monoclinic, $P2_1/c$
$a = 18.458$ (2) Å
$b = 6.5665$ (7) Å
$c = 13.8915$ (15) Å
$\beta = 91.111$ (2)°
$V = 1683.4$ (3) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.33$ mm^{-1}
$T = 298$ (2) K
0.33 × 0.22 × 0.17 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.668$, $T_{max} = 0.806$
13908 measured reflections
3837 independent reflections
3241 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.091$
$S = 1.05$
3837 reflections
220 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9296 (15)	Cu1—O4	1.9539 (13)
Cu1—N1	1.9320 (16)	Cu1—N2	2.0675 (16)
O1—Cu1—N1	93.09 (6)	O1—Cu1—N2	166.21 (7)
O1—Cu1—O4	90.60 (6)	N1—Cu1—N2	84.63 (7)
N1—Cu1—O4	171.54 (6)	O4—Cu1—N2	93.55 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O3^{i}	0.93	2.46	3.284 (3)	148
C8—H8A···O3^{i}	0.97	2.54	3.439 (3)	153
C8—H8B···O4^{ii}	0.97	2.43	3.338 (3)	157

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $x, y+1, z$.

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}$(methyl C).

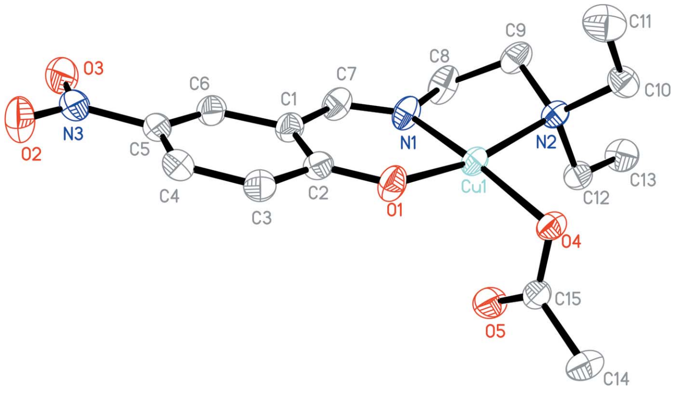


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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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References

Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
You, Z.-L. (2006). *Z. Anorg. Allg. Chem.* **632**, 669–674.
You, Z.-L., Han, X., Wang, J. & Niu, S.-Y. (2006). *Acta Cryst.* E**62**, m851–m853.
You, Z.-L., Jiao, Q.-Z., Niu, S.-Y. & Chi, J.-Y. (2006). *Z. Anorg. Allg. Chem.* **632**, 2481–2485.
You, Z.-L., Wang, J. & Han, X. (2006*a*). *Acta Cryst.* E**62**, m714–m716.
You, Z.-L., Wang, J. & Han, X. (2006*b*). *Acta Cryst.* E**62**, m860–m861.
You, Z.-L. & Zhu, H.-L. (2006). *Z. Anorg. Allg. Chem.* **632**, 140–146.