Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chlorido{2,4-dichloro-6-[(2-diethylamino-ethylimino)methyl]phenolato}copper(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.055
wR factor = 0.145
Data-to-parameter ratio = 19.3

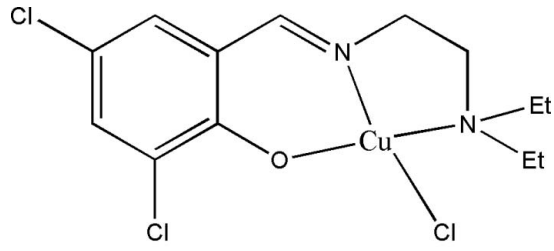
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 22 March 2007
Accepted 22 March 2007

In the title mononuclear copper(II) complex, [Cu($C_{13}H_{17}Cl_2N_2O$)Cl], the Cu^{II} ion is four-coordinated by one Schiff base ligand and one chloride anion in a slightly distorted square-planar geometry.

Comment

Copper(II) complexes derived from Schiff base ligands are of interest with regard to their structures and applications in coordination chemistry and materials chemistry. Recently, we have reported the crystal structures of a few Schiff base metal complexes (You, Han *et al.*, 2006; You *et al.*, 2006*a*,*b*). 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 terminal Cl^- anion in a slightly distorted square-planar geometry. The bond lengths (Table 1) are comparable to those in other Schiff base–copper(II) complexes (You, 2006; You & Zhu, 2006; You, Jiao *et al.*, 2006). The two *trans* angles at the metal centre are 170.22 (15) and 173.11 (13)°; all other angles around Cu1 are close to 90°, ranging from 83.44 (16) to 94.56 (12)°, indicating a slightly distorted square-planar geometry for Cu1.

In the crystal structure, molecules are linked through intermolecular C—H···Cl hydrogen bonds (Table 2), forming a chain along the [101] direction.

Experimental

3,5-Dichloro-2-hydroxybenzaldehyde and *N*,*N*-diethylethane-1,2-diamine were available commercially and were used without further purification. 3,5-Dichloro-2-hydroxybenzaldehyde (0.1 mmol, 19.2 mg) and *N*,*N*-diethylethane-1,2-diamine (0.1 mmol, 11.6 mg) were dissolved in methanol (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 $CuCl_2·2H_2O$ (0.1 mmol, 17.0 mg) with stirring. The resulting mixture was stirred for a further 10 min at room temperature. After allowing the filtrate to stand in air for 8 d, blue needle-shaped crystals were formed.

Crystal data

$[Cu(C_{13}H_{17}Cl_2N_2O)Cl]$
M_r = 387.18
Monoclinic, $P2_1/n$
a = 7.2839 (18) Å
b = 11.939 (3) Å
c = 17.958 (4) Å
β = 93.687 (3)°
V = 1558.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.91 mm^{-1}
T = 298 (2) K
0.30 × 0.12 × 0.08 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.598, T_{max} = 0.862
12912 measured reflections
3537 independent reflections
2908 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.145
S = 1.16
3537 reflections
183 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.912 (3)	Cu1—N2	2.097 (4)
Cu1—N1	1.942 (4)	Cu1—Cl3	2.2310 (14)
O1—Cu1—N1	92.13 (15)	O1—Cu1—Cl3	90.81 (11)
O1—Cu1—N2	170.22 (15)	N1—Cu1—Cl3	173.11 (13)
N1—Cu1—N2	83.44 (16)	N2—Cu1—Cl3	94.56 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···Cl3^{i}	0.93	2.75	3.670 (6)	171

Symmetry code: (i) $x-\frac{1}{2}, -y-\frac{1}{2}, z-\frac{1}{2}$.

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

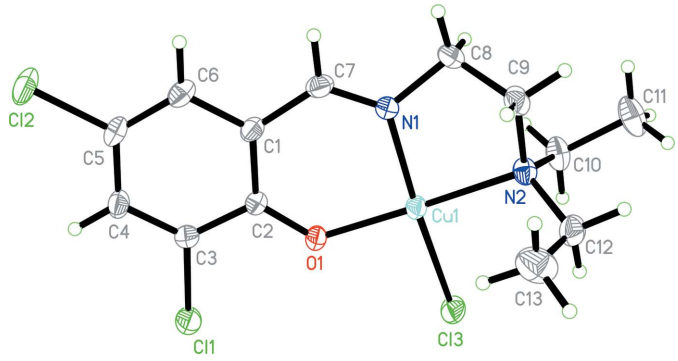


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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*.

This work was supported by the Scientific Research Foundation of the Education Office of Liaoning Province (Project No. 2005226).

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