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Azido{2,4-dichloro-6-[2-(diethylamino)-ethyliminomethyl]phenolato}copper(II)

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Key indicators

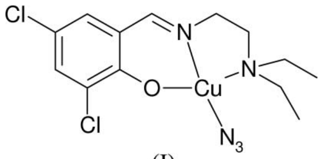
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.091
Data-to-parameter ratio = 16.8

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

In the mononuclear copper(II) compound, [Cu($C_{13}H_{17}Cl_2N_2O$)(N_3)], the Cu^{II} ion is four-coordinated by one imine N, one amine N, and one phenolate O atom of the Schiff base ligand, and by one terminal N atom of an azide anion, forming a distorted square-planar coordination.

Comment

Schiff base ligands have played an important role in the development of coordination chemistry as they readily form stable complexes with most transition metal ions (Pal *et al.*, 2005; Ueno *et al.*, 2004; Hou, 2005). During the last few years, there has been a great effort to identify the biological role of copper, primarily through techniques associated with the interface of biology/biochemistry/coordination chemistry (Collinson & Fenton, 1996; Hossain *et al.*, 1996; Tarafder *et al.*, 2002). It appears that the biological role of copper is primarily in redox reactions and as a biological catalyst, although much remains to be understood (Musie *et al.*, 2003; García-Raso *et al.*, 2003). An extensive effort has been made to prepare and characterize a variety of copper(II) coordination complexes in an attempt to model the physical and chemical behaviour of copper-containing enzymes (Reddy *et al.*, 2000). The peculiarity of copper lies in its ability to form complexes with coordination number four, five, and six (Ray *et al.*, 2003; Arnold *et al.*, 2003; Raptopoulou *et al.*, 1998). As part of our investigations in this area (Wei, 2005*a*,*b*), we report here a new mononuclear copper(II) complex, (I) (Fig. 1).


(I)

Complex (I) is a mononuclear copper(II) compound. The Cu^{II} ion is four-coordinated by one imine N, one amine N, and one phenolate O atom of a Schiff base ligand, and by one terminal N atom of an azide anion, forming a distorted square-planar coordination. All bond lengths are in normal ranges (Allen *et al.*, 1987). The bond lengths (Table 1) related to the Cu^{II} ion are comparable to the corresponding values observed in other Schiff base copper(II) complexes (Hebbachi & Benali-Cherif, 2005; Butcher *et al.*, 2003). The bond angles around the central metal ion show some deviations from ideal square-planar geometry, ranging from 84.35 (8) to 93.64 (7)°. The two *trans* bond angles are 164.30 (9) and 171.31 (7)°, respectively. In the crystal structure, the molecules are linked

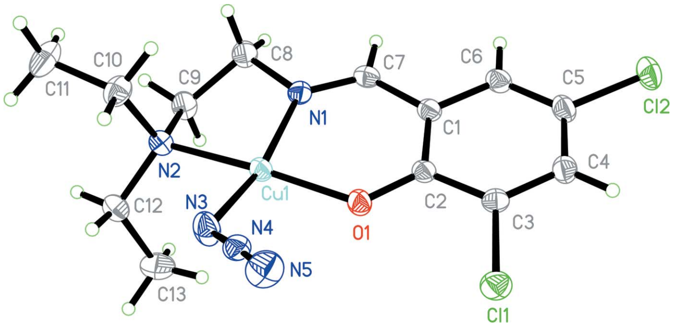


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

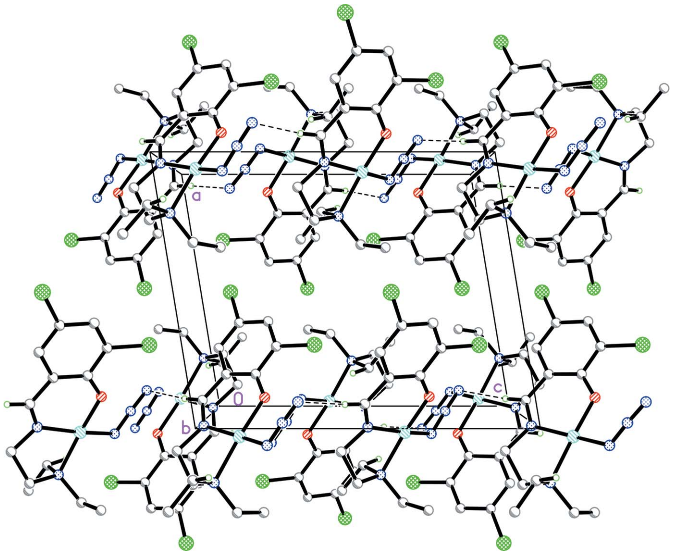


Figure 2
The crystal packing of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

through intermolecular C—H⋯N hydrogen bonds (Table 2), forming chains running along the *c* axis (Fig. 2).

Experimental

3,5-Dichlorosalicyaldehyde (1.0 mmol, 192.1 mg), *N*,*N*′-diethylethane-1,2-diamine (1.0 mmol, 116.2 mg), NaN_3 (1.0 mmol, 65.3 mg) and $Cu(CH_3COO)_2 \cdot H_2O$ (1.0 mmol, 199.1 mg) were dissolved in an MeOH solution (150 ml). The mixture was refluxed at at 340 K for about 1 h to give a clear blue solution. After keeping the cooled resulting solution in the dark for 8 d, blue block-shaped crystals were formed.

Crystal data

$[Cu(C_{13}H_{17}Cl_2N_2O)(N_3)]$
$M_r = 393.76$
Monoclinic, $P2_1/c$
$a = 10.723$ (2) Å
$b = 11.506$ (2) Å
$c = 13.192$ (3) Å
$\beta = 99.32$ (3)°
$V = 1606.1$ (6) Å^3
$Z = 4$
$D_x = 1.628$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5676 reflections
$\theta = 2.4$–27.3°
$\mu = 1.70$ mm^{-1}
$T = 298$ (2) K
Block, blue
0.37 × 0.18 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.572$, $T_{\max} = 0.822$
7787 measured reflections
3383 independent reflections
2882 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.024$
$\theta_{\max} = 27.0°$
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.091$
$S = 1.07$
3383 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.0366P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.34$ e Å^{-3}
$\Delta\rho_{\min} = -0.55$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.891 (2)	Cu1—N3	1.945 (2)
Cu1—N1	1.933 (2)	Cu1—N2	2.066 (2)
O1—Cu1—N1	93.64 (7)	O1—Cu1—N2	171.31 (7)
O1—Cu1—N3	92.56 (8)	N1—Cu1—N2	84.35 (8)
N1—Cu1—N3	164.30 (9)	N3—Cu1—N2	91.55 (8)

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C7—H7⋯N5^{i}	0.93	2.53	3.448 (3)	168
C10—H10*B*⋯N3	0.97	2.61	3.149 (3)	115

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

All 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 $U_{\rm iso}({\rm H}) = 1.2$ or $1.5U_{\rm eq}({\rm C})$.

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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