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{2,4-Dichloro-6-[2-(dimethylamino)ethylimino-methyl]phenolato}thiocyanatocopper(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.048
wR factor = 0.115
Data-to-parameter ratio = 16.2

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

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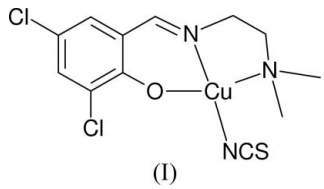
The title compound, $[Cu(C_{11}H_{12}Cl_2N_2O)(NCS)]$, is a mononuclear Schiff base copper(II) complex. The Cu^{II} atom is coordinated by one O and two N atoms of the Schiff base ligand, and by one N atom of the thiocyanate ligand, forming a square-planar coordination. The molecule possesses crystallographic mirror symmetry, with one disordered CH_2 group.

Comment

Schiff base complexes are of great interest in coordination chemistry (Goswami & Eichhorn, 1999; Dominguez-Vera *et al.*, 1998; Bernardo *et al.*, 1996). As an extension of our work on the structural characterization of Schiff base complexes (You, 2005*a*,*b*,*c*,*d*,*e*), the title Schiff base copper(II) complex, (I), is reported.



(I)

Complex (I) is a mononuclear copper(II) compound (Fig. 1). The Cu atom is four-coordinated in a square-planar geometry by one O and two N atoms of the Schiff base ligand, and by one N atom of the thiocyanate anion. The molecule possesses mirror symmetry, with atoms Cu1, Cl1, Cl2, S1, O1, N1, N2, N3, C1–C8, C12, H4, H6 and H7 lying on the crystallographic mirror plane. Atom C9 and its attached H atoms are disordered across the mirror plane. The values of the *trans*

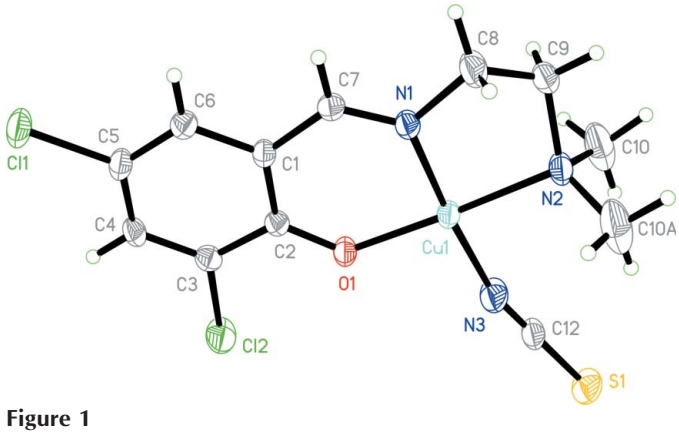


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The atom labelled with the suffix A is at the symmetry position $(x, \frac{1}{2}-y, z)$. Only one component of the disordered C9 group is shown.

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angles in the $CuON_3$ square plane are 175.66 (16) and 177.06 (14)°, indicating a slightly distorted square-planar coordination. The Cu—O and Cu—N bond lengths (Table 1) are comparable to the corresponding values observed in other Schiff base copper(II) complexes (MacLachlan *et al.*, 1996; Colacio *et al.*, 2000) and, as expected, the bond involving amine atom N2 [2.050 (4) Å] is longer than that involving imine atom N1 [1.927 (4) Å] (Mondal *et al.*, 2001). The crystal packing is shown in Fig. 2.

Experimental

3,5-Dichlorosalicylaldehyde (0.1 mmol, 19.0 mg) and *N*,*N*-dimethylethane-1,2-diamine (0.1 mmol, 8.8 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 20 min to give a yellow solution. To this solution was added an aqueous solution (2 ml) of NH_4NCS (0.1 mmol, 6.5 mg) and an MeOH solution (3 ml) of $Cu(CH_3COO)_2{\cdot}H_2O$ (0.1 mmol, 19.9 mg), with stirring. The mixture was stirred for another 20 min at room temperature. The filtrate was kept in air for 17 d, during which time blue block-shaped crystals were formed.

Crystal data

$[Cu(C_{11}H_{12}Cl_2N_2O)(NCS)]$
M_r = 381.75
Orthorhombic, *Pnma*
a = 19.301 (2) Å
b = 6.950 (1) Å
c = 11.173 (1) Å
V = 1498.8 (3) Å^3
Z = 4
D_x = 1.692 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1964 reflections
θ = 2.8–21.2°
μ = 1.95 mm^{-1}
T = 298 (2) K
Block, blue
0.23 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.663, T_{max} = 0.720
12536 measured reflections
1960 independent reflections
1486 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 28.3°
$h = -25 \rightarrow 24$
$k = -9 \rightarrow 9$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.115
S = 1.02
1960 reflections
121 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 1.0678P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.912 (3)	Cu1—N3	1.930 (4)
Cu1—N1	1.927 (4)	Cu1—N2	2.050 (4)
O1—Cu1—N1	92.49 (14)	O1—Cu1—N2	177.06 (14)
O1—Cu1—N3	91.85 (16)	N1—Cu1—N2	84.56 (15)
N1—Cu1—N3	175.66 (16)	N3—Cu1—N2	91.10 (17)

All non-H atoms except C9 and C10 lie on a crystallographic mirror plane. Atom C9 is disordered across the mirror plane and as a result the occupancy factor for the disordered components were fixed at 0.50 each. The 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) = 1.2 or 1.5U_{eq}(C). A short H9*A*···H10*B* contact of 1.82 Å is observed. A similar contact is also observed when the structure is refined in the non-centrosymmtric space group $Pna2_1$, which results in an *R* factor of 0.051 and inversion twinning, indicating that Pnma is the correct space group..

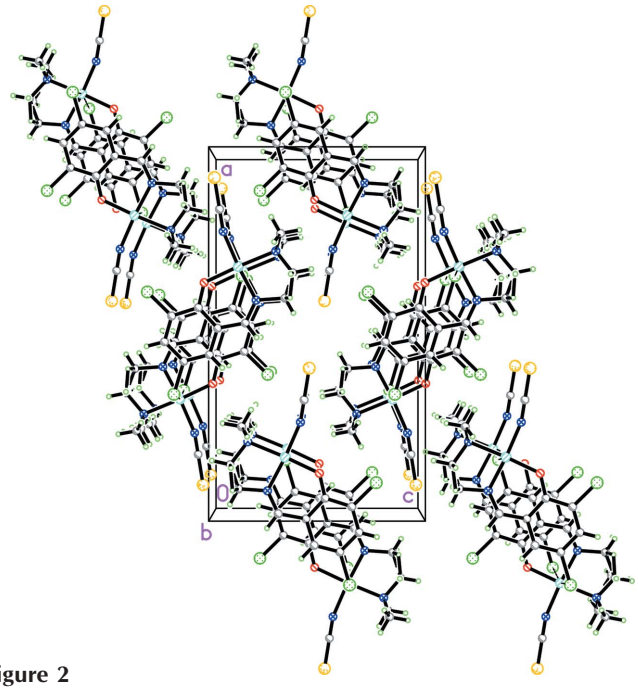

Figure 2
The packing of (I), viewed along the *b* axis.

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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