

Dichloro{4-chloro-2-[2-(isopropylamino)-ethyliminomethyl]phenolato}copper(II)

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In the title mononuclear copper(II) complex, $[\text{CuCl}_2(\text{C}_{12}\text{H}_{17}\text{ClN}_2\text{O})]$, the Cu^{II} atom is coordinated by one O atom and one imine N atom of a Schiff base ligand, and by two Cl^- anions, forming a slightly distorted tetrahedral geometry. In the crystal structure, molecules are linked through intermolecular hydrogen bonds, forming layers parallel to the bc plane.

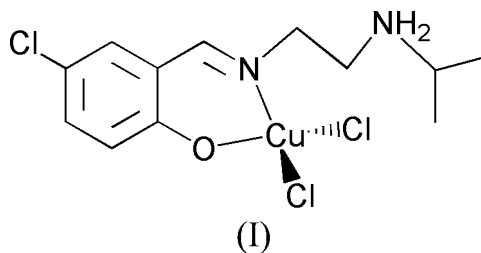
Key indicators

Single-crystal X-ray study
 $T = 298 \text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
 R factor = 0.032
 wR factor = 0.083
Data-to-parameter ratio = 21.8

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

Comment

Copper(II) complexes derived from Schiff base ligands have been studied extensively due to their interesting structures and wide applications (Bhaduri *et al.*, 2003; Rospendowski & Smith, 1988; Dominguez-Vera *et al.*, 1998; Hebbachi & Benali-Cherif, 2005; Butcher *et al.*, 2003). The present author has recently reported a related copper(II) complex (Hou, 2006) and, in a further investigation of such complexes, the structure of the title mononuclear copper(II) complex, (I), is reported here.

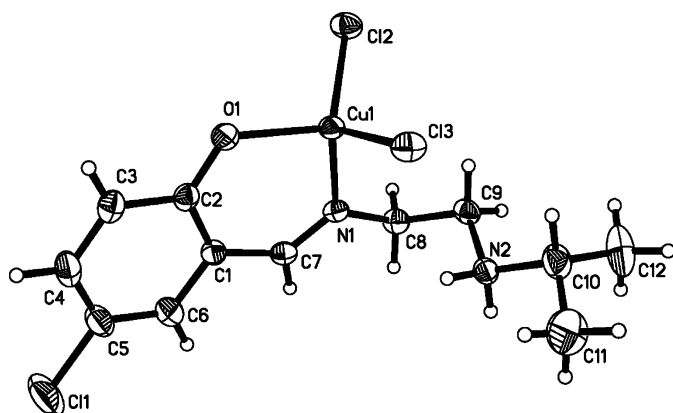


The Cu^{II} atom in (I) is in a slightly distorted tetrahedral geometry and is four-coordinated by one O atom and one imine N atom of a Schiff base ligand, and by two Cl^- anions (Fig. 1). The bond lengths (Table 1) involving the Cu^{II} atom are within normal ranges and comparable with the values observed in other similar copper(II) complexes (Shii *et al.*, 1999; Pal *et al.*, 2005; Colacio *et al.*, 1998).

In the crystal structure of (I), the molecules are linked through $\text{N}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{Cl}$ intermolecular hydrogen bonds (Table 2), forming layers parallel to the bc plane (Fig. 2).

Experimental

5-Chlorosalicylaldehyde (0.5 mmol, 78.3 mg), *N*-isopropylethane-1,2-diamine (0.5 mmol, 51.9 mg), and $\text{CuCl}_2\cdot 2\text{H}_2\text{O}$ (0.5 mmol, 85.2 mg) were dissolved in methanol (50 ml). The mixture was stirred at 328 K for 1 h to give a dark-blue solution. After keeping the solution in air for 11 d, blue block-shaped crystals of (I) were formed.


Figure 1

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

Crystal data

[CuCl₂(C₁₂H₁₇ClN₂O)]

M_r = 375.17

Monoclinic, *P*2₁/*c*

a = 11.887 (1) Å

b = 11.557 (1) Å

c = 12.531 (1) Å

β = 111.521 (1)°

V = 1601.5 (2) Å³

Z = 4

D_x = 1.556 Mg m⁻³

Mo *K*α radiation

μ = 1.86 mm⁻¹

T = 298 (2) K

Block, blue

0.22 × 0.18 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.686, *T_{max}* = 0.794

13689 measured reflections

3800 independent reflections

2981 reflections with *I* > 2σ(*I*)

R_{int} = 0.029

θ_{max} = 28.5°

Refinement

Refinement on *F*²

R[*F*² > 2σ(*F*²)] = 0.032

wR(*F*²) = 0.083

S = 1.05

3800 reflections

174 parameters

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.037*P*)² + 0.2985*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/*σ*)_{max} < 0.001

Δρ_{max} = 0.37 e Å⁻³

Δρ_{min} = -0.36 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

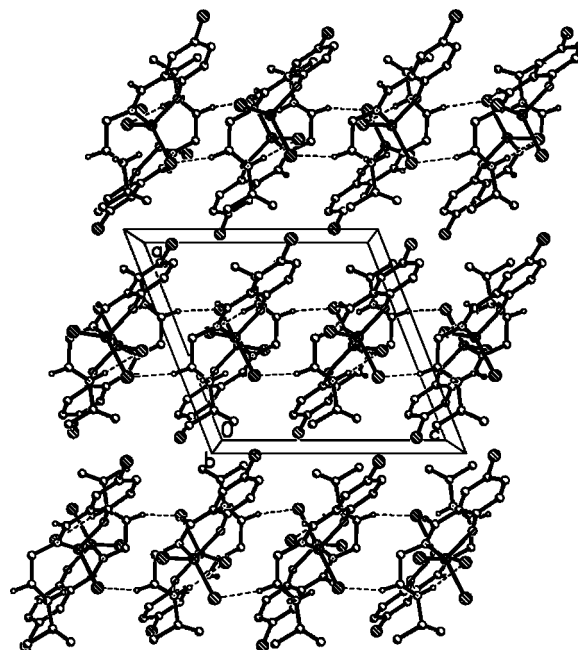
Cu1—O1	1.944 (2)	Cu1—Cl2	2.220 (1)
Cu1—N1	1.996 (2)	Cu1—Cl3	2.246 (1)
O1—Cu1—N1	97.62 (6)	O1—Cu1—Cl3	109.85 (5)
O1—Cu1—Cl2	108.51 (5)	N1—Cu1—Cl3	111.40 (5)
N1—Cu1—Cl2	110.10 (5)	Cl2—Cu1—Cl3	117.50 (3)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
N2—H2A⋯O1 ⁱ	0.90	1.98	2.828 (2)	157
N2—H2B⋯Cl2 ⁱ	0.90	2.47	3.2532 (19)	145
C7—H7⋯Cl3 ⁱ	0.93	2.77	3.619 (2)	153
C9—H9A⋯Cl3 ⁱⁱ	0.97	2.80	3.662 (2)	149

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


Figure 2

The crystal packing of (I), viewed along the *b* axis. Hydrogen bonds are indicated as dashed lines. Only H atoms involved in the hydrogen bonds have been included.

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and N—H = 0.90 Å, and with *U*_{iso}(H) = 1.2 or 1.5*U*_{eq}(C,N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; 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

- Bhaduri, S., Tasiopoulos, A. J., Bolcar, M. A., Abbound, K. A., Streib, W. E. & Christou, G. (2003). *Inorg. Chem.* **42**, 1483–1492.
- Bruker (1998). *SMART* (Version 5.628) and *SAINTE* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
- Butcher, R. J., Mockler, G. M. & McKern, O. (2003). *Acta Cryst.* **E59**, m1104–m1106.
- Colacio, E., Dominguez-Vera, J. M., Ghazi, M., Kivekäs, R., Klinga, M. & Moreno, J. M. (1998). *Inorg. Chem.* **37**, 3040–3045.
- Dominguez-Vera, J. M., Camara, F., Moreno, J. M., Colacio, E. & Stoeckli-Evans, H. (1998). *Inorg. Chem.* **37**, 3046–3050.
- Hebbachi, R. & Benali-Cherif, N. (2005). *Acta Cryst.* **E61**, m1188–m1190.
- Hou, H.-N. (2006). *Acta Cryst.* **E62**, m1533–m1534.
- Pal, S., Barik, A. K., Gupta, S., Hazra, A., Kar, S. K., Peng, S.-M., Lee, G.-H., Butcher, R. J., El Fallah, M. S. & Ribas, J. (2005). *Inorg. Chem.* **44**, 3880–3889.
- Rospondowski, B. & Smith, W. E. (1988). *Inorg. Chem.* **27**, 4509–4511.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Shii, Y., Motoda, Y., Matsuo, T., Kai, F., Nakashima, T., Tuchagues, J.-P. & Matsumoto, N. (1999). *Inorg. Chem.* **38**, 3513–3522.