metal-organic papers

Dichlorobis[2-(o-tolyliminomethyl)phenolato]-copper(II)

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The title compound, [Cu(C$_{14}$H$_{13}$NO)$_2$Cl$_2$], is a mononuclear copper(II) complex of a Schiff base. The Cu^{II} atom is coordinated by two O atoms from two 2-(o-tolyliminomethyl)phenolate ligands, and by two chloride anions, forming a tetrahedral geometry.
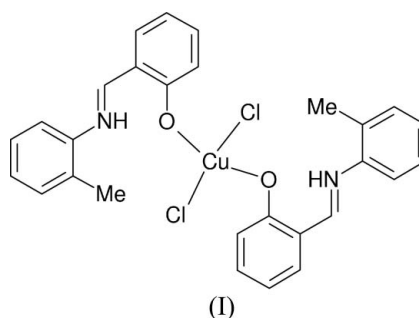
Comment

Copper(II) complexes are of great interest in coordination chemistry (Wagner & Walker, 1983; Margeat *et al.*, 2004). As an extension of work on the structural characterization of copper compounds, the title mononuclear copper(II) complex, (I) (Fig. 1), is reported.

(I)

The Cu atom is in a tetrahedral geometry (Table 1) and is coordinated by two O atoms from two 2-(o-tolyliminomethyl)phenolate ligands, and by two chloride anions. The Cu—O and Cu—Cl bond lengths are comparable to the values observed in other copper(II) complexes (MacLachlan *et al.*, 1996; Countryman *et al.*, 1974). There are no short intermolecular contacts (Fig. 2). Intramolecular hydrogen bonds are found in the ligands (Fig. 1 and Table 2).
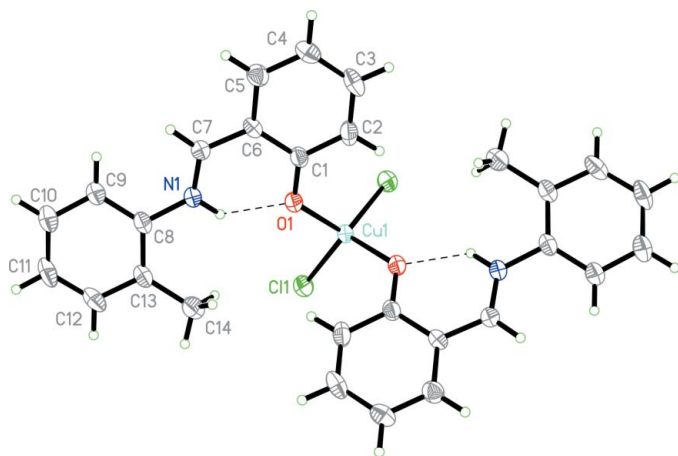
Experimental

o-Tolylamine (0.1 mmol, 10.7 mg), salicylaldehyde (0.1 mmol, 12.2 mg) and Cu(CH$_3$COO)$_2$·H$_2$O (0.1 mmol, 20.0 mg) were dissolved in methanol (15 ml). The mixture was stirred for 1 h and filtered. After keeping the filtrate in air for 7 d, blue block-shaped crystals were formed.

Crystal data

[Cu(C$_{14}$H$_{13}$NO)$_2$Cl$_2$]	$D_x = 1.443$ Mg m^{-3}
$M_r = 556.95$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 726
$a = 16.043$ (3) Å	reflections
$b = 10.536$ (2) Å	$\theta = 2.3–22.2°$
$c = 15.647$ (3) Å	$\mu = 1.09$ mm^{-1}
$\beta = 104.31$ (3)°	$T = 293$ (2) K
$V = 2562.8$ (9) Å^3	Block, blue
$Z = 4$	$0.32 \times 0.28 \times 0.27$ mm

Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

Data collection

Bruker SMART CCD area-detector diffractometer	2847 independent reflections
ω scans	1462 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan	$R_{int} = 0.073$
(*SADABS*; Sheldrick, 1996)	$\theta_{max} = 27.5°$
$T_{min} = 0.722$, $T_{max} = 0.758$	$h = -16 \rightarrow 20$
8015 measured reflections	$k = -13 \rightarrow 13$
	$l = -20 \rightarrow 18$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.057$	
$wR(F^2) = 0.138$	
$S = 0.95$	$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2]$
2847 reflections	where $P = (F_o^2 + 2F_c^2)/3$
163 parameters	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 0.43$ e Å^{-3}
	$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.980 (3)	Cu1—Cl1	2.238 (2)
O1^i—Cu1—O1	102.89 (17)	O1—Cu1—Cl1	106.04 (9)
O1^i—Cu1—Cl1	115.89 (9)	Cl1—Cu1—Cl1^i	110.23 (8)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O1	0.90 (1)	1.91 (4)	2.593 (4)	132 (4)

Atom H1 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$. The data are relatively weak, with almost half the reflections classed as 'unobserved'.
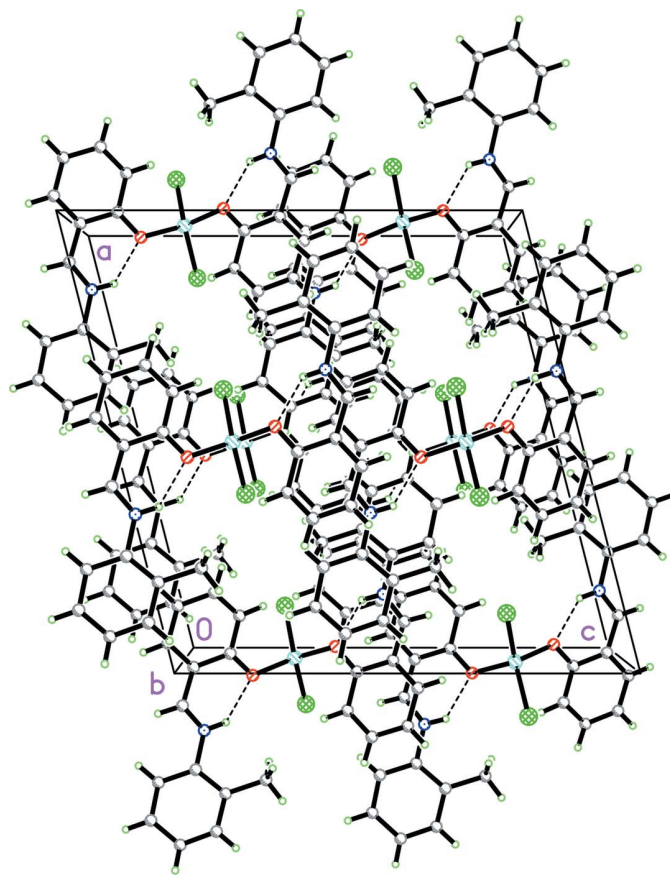
Figure 2
The crystal packing of (I), viewed along the *a* axis. Intramolecular hydrogen bonds are shown as dashed lines.

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