Chloro{2-[tris(hydroxymethyl)methyliminomethyl]-phenolato}copper(II)

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In the title compound, $[Cu(C_{11}H_{14}NO_4)Cl]$, the tridentate Schiff base ligand coordinates to the metal atom through the N and O atoms, forming a square-planar coordination geometry.

Comment

The chemistry of transition metal ion complexes of hydroxy (aryl and alkyl OH) rich molecules containing imine/amine groups is important in biomimetic chemistry (Cornman *et al.*, 1992). Many complexes of this kind have been reported (Asgedom & Rao, 1996; Dey, Rao, Saarenketo & Rissanen, 2002; Dey, Rao, Saarenketo, Rissanen & Kolehmainen, 2002). We report here a new copper(II) complex, (I), with a tridentate Schiff base ligand.
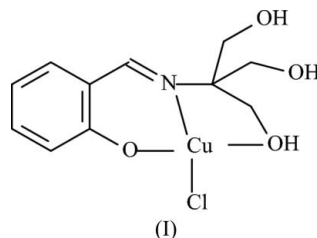
In compound (I), the Cu^{II} center is four-coordinated in a square-planar configuration by one N and two O atoms of the Schiff base ligand and one Cl atom. The Cu—O bond lengths
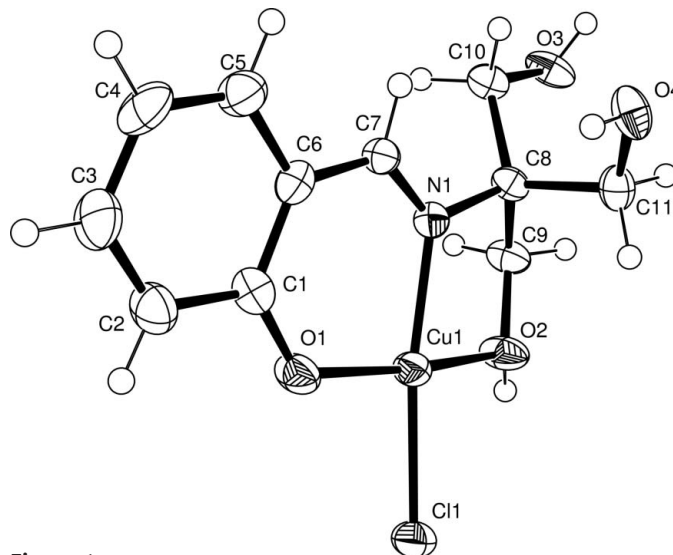

Figure 1
An *ORTEPII* plot (Johnson, 1976) of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

are 1.885 (2) and 1.979 (2) Å; the shorter distance between copper and the phenoxy O atom indicates that the electronegativity of atom O1 is stronger than that of the other O atoms of the ligand.

Experimental

The ligand 2-[tris(hydroxymethyl)methyliminomethyl]phenol was prepared according to the literature procedure of Asgedom *et al.* (1996). Cuprous chloride (0.105 g, 0.5 mmol) was added to a solution of the ligand (0.111 g, 0.5 mmol) in water (10 ml). After stirring for a short time, the solution turned dark green. The filtrate was left for 2 d at room temperature and green needle-shaped crystals were obtained in about 62% yield.

Crystal data

$[Cu(C_{11}H_{14}NO_4)Cl]$	Mo $K\alpha$ radiation
$M_r = 323.22$	Cell parameters from 1879
Tetragonal, $P\bar{4}2_1c$	reflections
$a = 16.7345$ (6) Å	$\theta = 2.4–23.3°$
$c = 8.7634$ (6) Å	$\mu = 2.00$ mm^{-1}
$V = 2454.1$ (2) Å^3	$T = 293$ (2) K
$Z = 8$	Needle, green
$D_x = 1.750$ Mg m^{-3}	$0.21 \times 0.09 \times 0.07$ mm

Data collection

Bruker APEX area-dectector diffractometer	2918 independent reflections
φ and ω scans	2661 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$R_{int} = 0.049$
$T_{min} = 0.679$, $T_{max} = 0.873$	$\theta_{max} = 27.9°$
20984 measured reflections	$h = -21 \rightarrow 21$
	$k = -21 \rightarrow 21$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 1.812P]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.077$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.36$ e Å^{-3}
2918 reflections	$\Delta\rho_{min} = -0.21$ e Å^{-3}
165 parameters	Absolute structure: Flack (1983), 1265 Friedel pairs
H-atom parameters constrained	Flack parameter: 0.007 (15)

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.885 (2)	Cu1—O2	1.979 (2)
Cu1—N1	1.951 (2)	Cu1—Cl1	2.2366 (8)
O1—Cu1—N1	94.92 (10)	O1—Cu1—Cl1	93.56 (7)
O1—Cu1—O2	169.50 (10)	N1—Cu1—Cl1	171.25 (8)
N1—Cu1—O2	81.81 (10)	O2—Cu1—Cl1	90.22 (7)

H atoms were placed in idealized positions [N—H = 0.82 Å, C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$] and were included in the refinement in the riding-model approximation.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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