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Key indicators

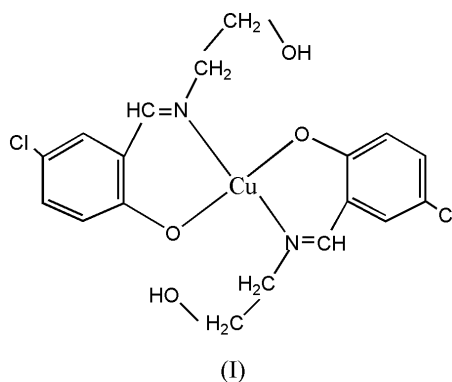
Single-crystal X-ray study
 $T = 193\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.029
 wR factor = 0.071
Data-to-parameter ratio = 15.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis[4-chloro-2-(2-hydroxyethyliminomethyl)-
phenolato- $\kappa^2\text{N,O}$]copper(II)

A new copper(II) complex, $[\text{Cu}(\text{C}_9\text{H}_9\text{ClNO}_2)_2]$, has been synthesized by the reaction of a tridentate Schiff base ligand derived from 5-chlorosalicylaldehyde and 2-ethanolamine with $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$. The Cu atom lies on a center of symmetry; the asymmetric unit is thus one half-molecule. The coordination geometry around the metal atom is square-planar, with the Schiff base ligand coordinated through two N and two O atoms in a *trans* configuration.

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Comment

Schiff base complexes of copper have been intensively studied as mimics of copper proteins, exhibiting diversity of geometric and electronic structures, and very good catalytic activity in reactions of molecular oxygen (Holland & Tolman, 1999; Fenton, 1999). Ligands derived from salicylidene-2-ethanolamine have previously been incorporated into a number of mono- and dinuclear transition metal complexes, in addition to tetranuclear Fe^{II} and Cu^{II} clusters with cubane structures (Colette *et al.*, 2002; Oshio *et al.*, 2000). We report here the X-ray crystal structure of the title compound, (I).



The bond lengths and angles in (I) are listed in Table 1. The Cu atom lies on a center of symmetry; the asymmetric unit is thus one half-molecule. The metal atom is coordinated by Schiff base ligands through two N and two O atoms in a *trans* configuration, where the Schiff base ligand is a monoanion with the OH group deprotonated. The O—Cu—O and N—Cu—N angles are 180° . Therefore, the geometry of the Cu^{II} ion is square planar (Fig. 1). The molecular packing diagram (Fig. 2) reveals an interaction between the metal atom and the hydroxy O atom, and intermolecular C7—H7 \cdots Cl1 and C8—H8A \cdots Cl1 hydrogen bonds (Table 2), resulting in a three-dimensional network structure. An intramolecular O2—H2 \cdots O1 hydrogen bond (Table 2) also exists in the complex.

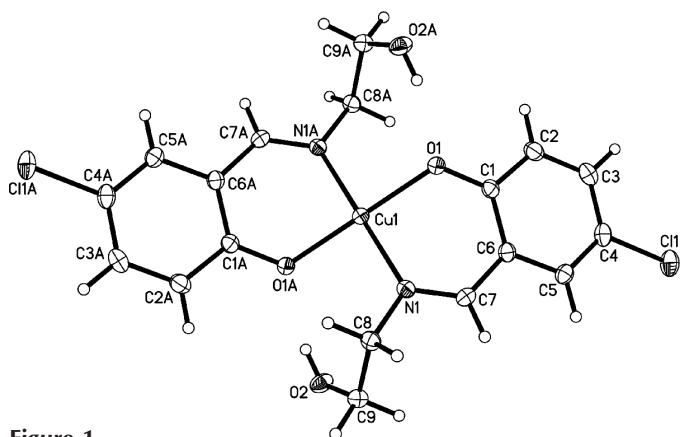


Figure 1
The molecular structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme. The suffix A corresponds to symmetry code (i) in Table 1.

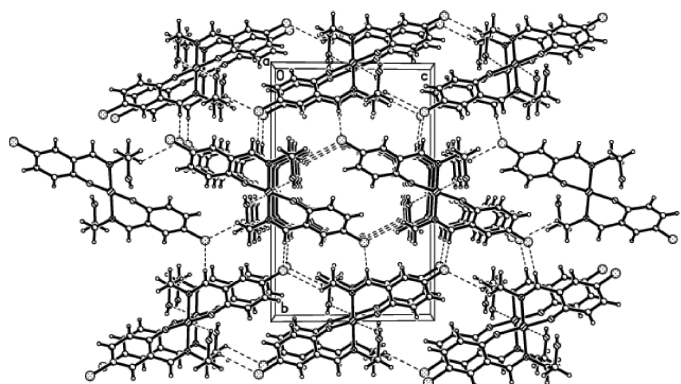


Figure 2
The molecular packing diagram of (I). The dashed lines indicate hydrogen bonds.

Experimental

The title compound, (I), was prepared by reacting $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$ with 5-chlorosalicylaldehyde and 2-ethanolamine (1:1:1) in ethanol. Single crystals of (I) suitable for X-ray study were obtained by recrystallization from dimethylformamide.

Crystal data

$[\text{Cu}(\text{C}_9\text{H}_9\text{ClNO}_2)_2]$
 $M_r = 460.78$
 Monoclinic, $P2_1/n$
 $a = 4.9589$ (12) Å
 $b = 16.872$ (4) Å
 $c = 10.711$ (2) Å
 $\beta = 94.530$ (5)°
 $V = 893.4$ (3) Å³
 $Z = 2$

$D_x = 1.713$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 3969 reflections
 $\theta = 3.1$ – 27.5 °
 $\mu = 1.55$ mm⁻¹
 $T = 193$ (2) K
 Block, brown–yellow
 $0.30 \times 0.25 \times 0.10$ mm

Data collection

Rigaku Mercury diffractometer
 ω scans
 Absorption correction: multi-scan (Jacobson, 1998)
 $T_{\min} = 0.654$, $T_{\max} = 0.860$
 9835 measured reflections
 2041 independent reflections

1891 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 $\theta_{\text{max}} = 27.5$ °
 $h = -6 \rightarrow 6$
 $k = -21 \rightarrow 21$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.071$
 $S = 1.12$
 2041 reflections
 129 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 0.5395P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.50 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1–O1	1.9540 (13)	Cu1–N1	1.9961 (15)
O1 ⁱ –Cu1–O1	180	O1–Cu1–N1	89.01 (6)
O1 ⁱ –Cu1–N1 ⁱ	89.01 (6)	N1 ⁱ –Cu1–N1	180

Symmetry code: (i) $1 - x, 1 - y, -z$.

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C7–H7 \cdots Cl1 ⁱⁱ	0.95	2.89	3.8144 (19)	165
C8–H8A \cdots Cl1 ⁱⁱⁱ	0.99	2.86	3.446 (2)	119
O2–H2 \cdots O1 ⁱ	0.81 (3)	1.87 (3)	2.658 (2)	167 (3)

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

H atoms attached to C were included in calculated positions, with C–H distances ranging from 0.95 to 0.99 Å. The H atoms were then included in the refinement in riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atom attached to atom O2 was located in a difference density map and refined isotropically.

Data collection: *CrystalClear* (Pflugrath, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MS, 2000–2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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