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[*N*,*N*′-Bis(3-methylsalicylidene)propane-1,3-diaminato]copper(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.010 Å
R factor = 0.067
wR factor = 0.175
Data-to-parameter ratio = 18.0

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

In the title mononuclear complex, $[Cu(C_{19}H_{20}N_2O_2)]$, the four-coordinate Cu^{II} atom is in a distorted square-planar geometry defined by the two N atoms and two O atoms of the Schiff base ligand.

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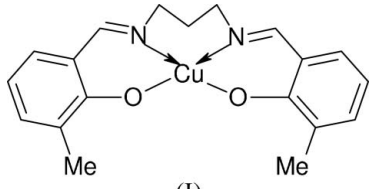
Comment

N,*N*′-Bis(salicylidene)-1,3-diaminopropane is a versatile tetradentate ligand that forms complexes with a large number of transition metal ions (You, Zhu & Liu, 2004; You & Zhu, 2004). However, the complexes of the methyl-substituted analogue, *N*,*N*′-bis(3-methylsalicylidene)-1,3-diaminopropane, have rarely been studied. Interest in such Schiff base complexes stems from their properties and unusual solid-state structures (Koner *et al.*, 2003; Palopoli *et al.*, 2000). We have focused our attention on the synthesis of transition metal complexes of flexible ligands as they are expected to adopt motifs that can be predicted by the geometric requirements of the metal ions (You *et al.*, 2005; You, Xiong & Zhu, 2004).



(I)

Complex (I) is a mononuclear copper(II) compound (Fig. 1). The Cu^{II} atom is four-coordinate, in a distorted

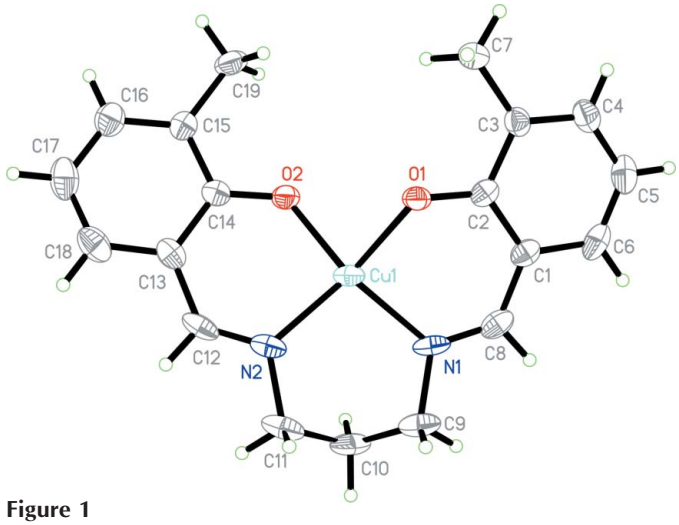


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

square-planar environment defined by the two N atoms and two O atoms of the deprotonated Schiff base ligand. The Cu—O and Cu–N bond lengths are similar to distances observed in other Schiff base copper(II) complexes (Deschamps *et al.*, 2003; Margeat *et al.*, 2004; You, 2005). The *trans* angles in the CuO_2N_2 square plane deviate from linearity by 17.77 (18) and 19.91 (17)°; the dihedral angle between the two benzene rings is 22.1 (2)°. The conformation of the six-membered chelate ring made up of the metal, azomethine N atoms and three C atoms of the connecting 1,3-diaminopropane is that of a chair.

Experimental

3-Methylsalicylaldehyde (0.2 mmol, 27.2 mg) and 1,3-diaminopropane (0.1 mmol, 7.4 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a yellow solution. To the solution was added a MeOH solution of $Cu(CH_3COO)_2{\cdot}H_2O$ (0.1 mmol, 19.9 mg). The mixture was stirred for another 10 min at room temperature. After the filtrate had been allowed to stand for 11 d, blue block-shaped crystals deposited from solution.

Crystal data

$[Cu(C_{19}H_{20}N_2O_2)]$
M_r = 371.91
Monoclinic, $P2_1/c$
a = 10.328 (1) Å
b = 7.732 (1) Å
c = 23.656 (2) Å
β = 114.38 (1)°
V = 1720.6 (3) Å^3
Z = 4
D_x = 1.436 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2075 reflections
θ = 2.2–21.2°
μ = 1.28 mm^{-1}
T = 298 (2) K
Block, blue
0.35 × 0.28 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.663, T_{max} = 0.757
19004 measured reflections
3944 independent reflections
2182 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 27.5°
$h = -13 \rightarrow 13$
$k = -10 \rightarrow 10$
$l = -30 \rightarrow 30$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.175
S = 1.04
3944 reflections
219 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 2.5236P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.901 (3)	Cu1—N1	1.990 (5)
Cu1—O2	1.907 (4)	Cu1—N2	1.956 (5)
O1—Cu1—O2	83.82 (15)	O2—Cu1—N1	160.09 (17)
O1—Cu1—N1	90.28 (18)	O2—Cu1—N2	92.30 (19)
O1—Cu1—N2	162.23 (18)	N2—Cu1—N1	98.8 (2)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$. The H atoms of the methyl groups were rotated to fit the electron density. The highest electron-density peak is located 0.98 Å from atom Cu1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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