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[*o*-Phenylenebis(salicylideneaminato)]copper(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.011 Å
R factor = 0.076
wR factor = 0.171
Data-to-parameter ratio = 15.4

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

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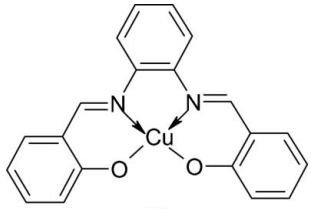
The title compound, $[Cu(C_{20}H_{14}N_2O_2)]$, is a mononuclear copper(II) compound, the Cu atom of which is coordinated by two N and two O atoms from the *o*-phenylenebis(salicylideneamine) ligand in a square-planar geometry.

Comment

The title mononuclear copper(II) complex, (I), was reported as an orthorhombic polymorph in 1996 (Suresh *et al.*, 1996). The compound also crystallizes as a monohydrate (Yao *et al.*, 1997). In this work, although the compound was recrystallized from methanol that should contain some water, only the anhydrous form was obtained, in a second orthorhombic form.



(I)

In the title complex (Fig. 1), the Cu atom exists in a square-planar geometry, as it is coordinated by two N and two O atoms from the ligand; the *trans* angles are nearly 180° (Table 1). The Cu—N and Cu—O bond lengths are comparable with those observed in other copper(II) complexes (MacLachlan *et al.*, 1996).

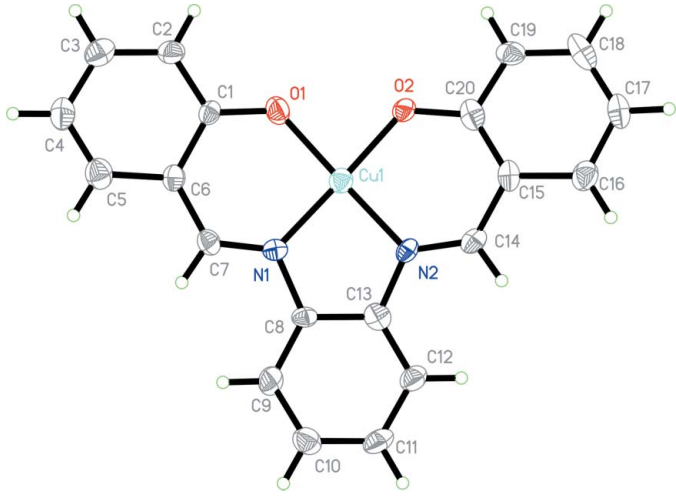


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

The molecules of (I) are held together only by van der Waals forces only (Fig. 2), which is similar to the orthorhombic polymorph reported by Suresh *et al.* (1996).

Experimental

o-Phenylenediamine (0.1 mmol, 10.8 mg), salicylaldehyde (0.2 mmol, 24.2 mg) and copper acetate hydrate (0.1 mmol, 20.0 mg) were dissolved in methanol (15 ml). The mixture was stirred for 1 h and filtered. Block-shaped crystals of (I) separated from the filtrate after 3 d.

Crystal data

$[Cu(C_{20}H_{14}N_2O_2)]$
M_r = 377.87
Orthorhombic, $P2_12_12_1$
a = 5.470 (1) Å
b = 16.618 (3) Å
c = 17.322 (3) Å
V = 1574.1 (7) Å^3
Z = 4
D_x = 1.594 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 880 reflections
θ = 2.0–21.3°
μ = 1.40 mm^{-1}
T = 298 (2) K
Block, blue
0.23 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.739, T_{max} = 0.817
9949 measured reflections
3487 independent reflections
2138 reflections with $I > 2\sigma(I)$
R_{int} = 0.096
θ_{max} = 27.5°
$h = -6 \rightarrow 7$
$k = -21 \rightarrow 20$
$l = -22 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.171
S = 1.03
3487 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.067P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack (1983), with 1385 Friedel pairs
Flack parameter: 0.07 (4)

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.844 (5)	Cu1—N1	1.856 (6)
Cu1—O2	1.847 (5)	Cu1—N2	1.869 (5)
O1—Cu1—O2	83.8 (2)	O1—Cu1—N2	178.7 (3)
O1—Cu1—N1	94.4 (2)	O2—Cu1—N2	95.0 (2)
O2—Cu1—N1	178.2 (2)	N1—Cu1—N2	86.8 (3)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

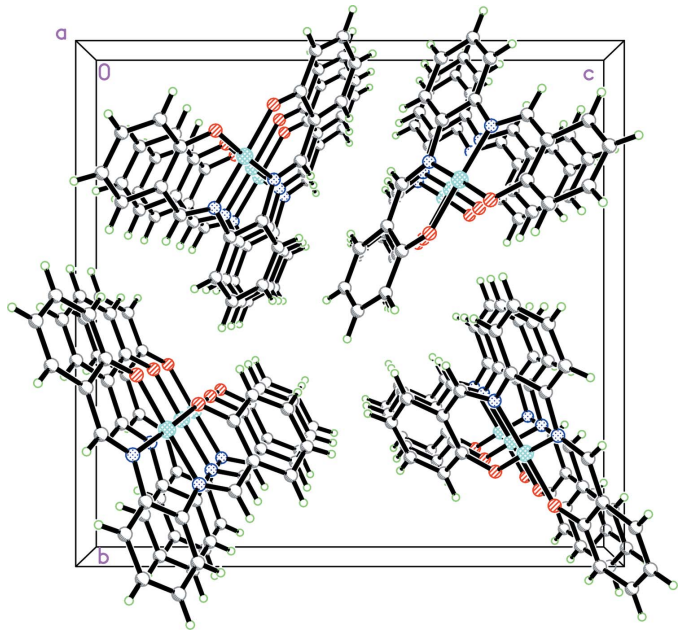


Figure 2
The crystal packing of (I), viewed along the *a* axis.

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