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Bis[2-(1-naphthyliminomethyl)phenolato-κ^2N,O]copper(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.015 Å
R factor = 0.067
wR factor = 0.176
Data-to-parameter ratio = 10.6

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

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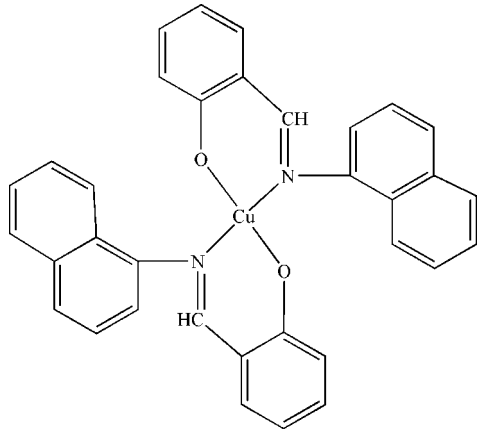
In the title complex, $[Cu(C_{17}H_{12}NO)_2]$, the Cu^{II} ion is coordinated by two bidentate ligands in a *trans* arrangement, forming a CuN_2O_2 slightly distorted square-planar configuration.

Comment

Schiff base complexes play an important role in stereochemical models of transition metal coordination chemistry, with their easy preparation, diversity and structural variation (Gamovski *et al.*, 1993). 2-Hydroxy Schiff base ligands and their copper(II) complexes play a major role in both synthetic and structural research (Maggio *et al.*, 1974). As part of a series of studies (Wang *et al.*, 2007), we report here the synthesis and crystal structure of the title compound, (I), a new copper(II) complex formed with a bidentate Schiff base ligand derived from the condensation of salicylaldehyde and 1-naphthylamine.



(I)

In the molecular structure of (I) (Fig. 1), the Cu^{II} ion is coordinated by two bidentate ligands in a *trans* arrangement. The bond lengths and angles (Table 1) show that the coordination geometry deviates slightly from square-planar. Details of similar crystal structures have been reported by Fernández-G. *et al.* (1998). The planes formed by atoms O1/O2/N1/N2/Cu1 (*A*), C2–C7 (*B*), C8–C17 (*C*), C19–C24 (*D*) and C25–C34 (*E*) make the following dihedral angles; *A*/*B* 19.53 (37)°, *A*/*C* 81.51 (13)°, *A*/*D* 22.84 (30)° and *A*/*E* 79.76 (14)°.

In the crystal structure, the only significant intermolecular interaction appears to be a single weak C—H$\cdots\pi$ interaction [H16$\cdots Cg^{i}$ = 2.86 Å, C16$\cdots Cg^{i}$ = 3.650 (13) Å and C16—H16$\cdots Cg^{i}$ = 144°; symmetry code: (i) 1 + x, y, z; Cg is the centroid of the C19–C24 ring].

Experimental

1-Naphthylamine (1 mmol, 143.2 mg) was dissolved in hot methanol (10 ml) and added dropwise to a methanol solution (3 ml) of salicylaldehyde (1 mmol, 0.11 ml). The mixture was then stirred at 323 K for 2 h. An aqueous solution (2 ml) of cupric acetate monohydrate (1 mmol, 199.7 mg) was then added dropwise and the mixture stirred for another 5 h. The solution was kept at room temperature for 10 d, whereupon crystals of (I) suitable for X-ray diffraction analysis were obtained.

Crystal data

$[Cu(C_{17}H_{12}NO)_2]$
M_r = 556.09
Monoclinic, *Pc*
a = 8.6600 (15) Å
b = 12.190 (2) Å
c = 12.496 (2) Å
β = 99.317 (2)°
V = 1301.7 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 298 (2) K
0.63 × 0.21 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.609, T_{max} = 0.887
6484 measured reflections
3714 independent reflections
2599 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.176
S = 1.01
3714 reflections
352 parameters
257 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Absolute structure: Flack (1983), with 1411 Friedel pairs
Flack parameter: 0.53 (3)

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.864 (6)	Cu1—N1	1.991 (9)
Cu1—O2	1.864 (5)	Cu1—N2	2.016 (9)
O1—Cu1—O2	178.7 (5)	O1—Cu1—N2	88.7 (3)
O1—Cu1—N1	91.5 (3)	O2—Cu1—N2	91.1 (3)
O2—Cu1—N1	88.6 (3)	N1—Cu1—N2	178.4 (5)

The value of the Flack (1983) parameter indicates that the crystal is an inversion twin. All H atoms were placed in geometrically calculated positions, with C—H = 0.93–0.97 Å, and allowed to ride on their respective parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

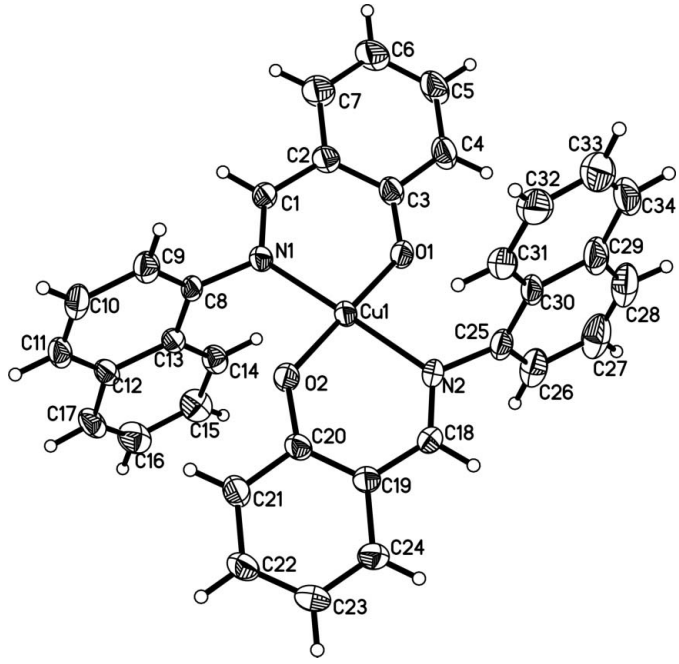


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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