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[*N*,*N*′-Bis(2-oxido-1-naphthylmethylene)-propane-1,3-diamine]copper(II)

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Key indicators

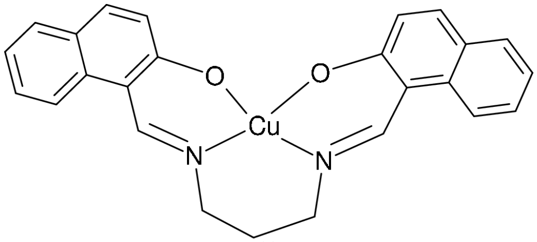
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.006 Å
R factor = 0.047
wR factor = 0.123
Data-to-parameter ratio = 14.8

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

The title compound, [Cu($C_{25}H_{20}N_2O_2$)], is a centrosymmetric mononuclear copper(II) complex. The Cu^{II} atom and central C atom of the propane linkage lie on a mirror plane. The Cu^{II} ion is coordinated by two N atoms and two O atoms from a bis-Schiff base ligand in a slightly distorted square-planar geometry.

Comment

Transition metal complexes are very important in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism, and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). As an extension of work on the structural characterization of copper(II) complexes, the title compound, (I), is reported here.



(I)

Complex (I) is a mononuclear copper(II) complex (Fig. 1). The asymmetric unit contains one half of the complex, with the other half being generated by crystallographic mirror symmetry; atoms Cu1 and C13 lie on the mirror plane. The central Cu^{II} ion is coordinated by two O atoms and two N atoms of the bis-Schiff base ligand. This CuO$_2$N$_2$ coordination has a slightly distorted square-planar geometry. The Cu atom is 0.016 (3) Å out of the mean plane of the four donor atoms. The Cu—O bond length [1.849 (3) Å; Table 1] is shorter than the value of 1.880 (2) Å observed in another Schiff base copper(II) complex (Burgess *et al.*, 2001). The Cu—N bond [1.875 (3) Å] is much shorter than the value of 2.009 (3) Å observed in the same complex. Both *trans* angles in the square plane of (I) are 173.63 (13)°, indicating a slightly distorted square-planar configuration of atom Cu1. The dihedral angle between the two naphthalene ring systems is 52.8 (5)°.

Experimental

1,3-Diaminopropane (0.2 mmol, 15.8 mg) and 2-hydroxy-1-naphthaldehyde (0.4 mmol, 68.9 mg) were dissolved in EtOH (15 ml). The mixture was stirred for 30 min to give a clear yellow solution. To this solution was added an EtOH solution (15 ml) of Cu(CH_3COO)$_2$·2H_2O (0.2 mmol, 43.6 mg), with stirring. The mixture was stirred for a further 30 min and filtered. The filtrate was allowed to stand at room temperature in air for 11 d, yielding blue block-shaped crystals of (I).

Crystal data

$[Cu(C_{25}H_{20}N_2O_2)]$
$M_r = 443.97$
Orthorhombic, $Cmc2_1$
$a = 30.614$ (6) Å
$b = 8.4578$ (17) Å
$c = 7.7462$ (15) Å
$V = 2005.7$ (7) Å^3
$Z = 4$
$D_x = 1.470$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 2010 reflections
$\theta = 2.5$–22.6°
$\mu = 1.11$ mm^{-1}
$T = 273$ (2) K
Block, blue
0.28 × 0.25 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.746$, $T_{max} = 0.825$
5705 measured reflections

2074 independent reflections
1845 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 26.5°$
$h = -38 \rightarrow 33$
$k = -10 \rightarrow 10$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.124$
$S = 1.01$
2074 reflections
140 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Absolute structure: Flack (1983); 932 Friedel pairs
Flack parameter = 0.11 (2)

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.849 (3)	Cu1—N1	1.875 (3)
O1^i—Cu1—O1	82.64 (16)	O1—Cu1—N1	91.06 (13)
O1^i—Cu1—N1	173.63 (13)	N1—Cu1—N1^i	95.2 (2)

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

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

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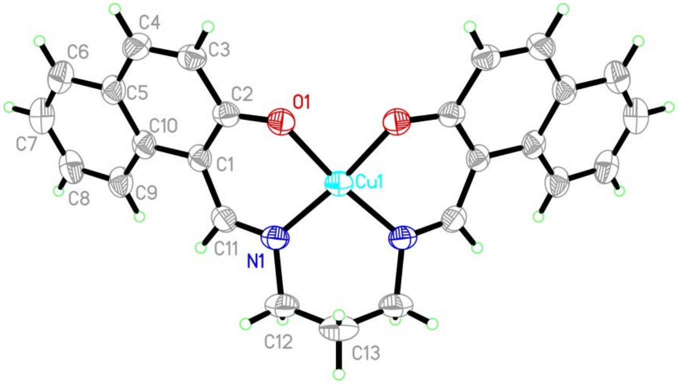

Figure 1
The structure of (I), showing the atomic numbering for the contents of the asymmetric unit. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by $1 - x, y, z$.

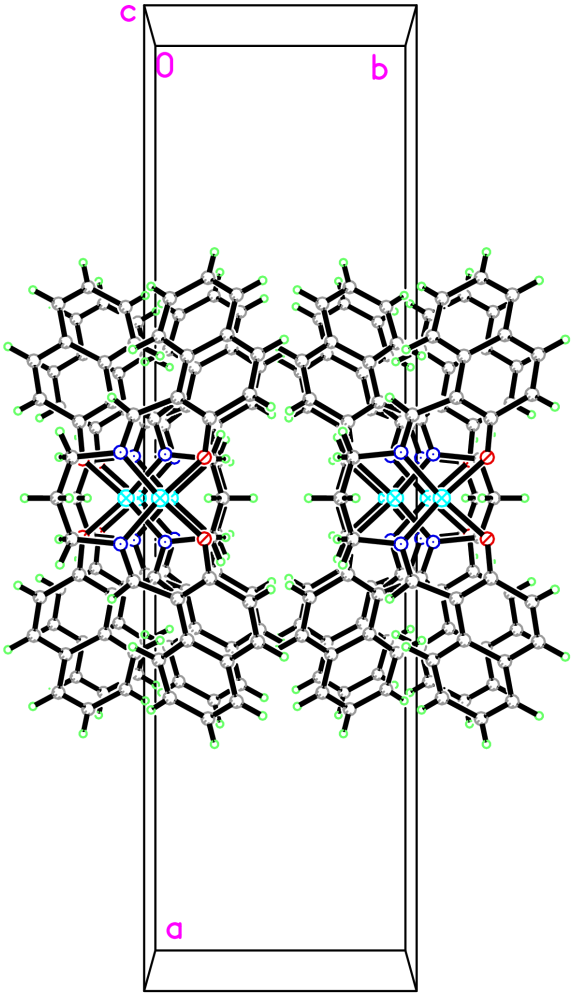

Figure 2
Part of the crystal packing of (I), viewed along the *c* axis.

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