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[*N*,*N*′-Bis(2-oxidonaphthylmethylidene)-ethane-1,2-diamine-κ^4O,N,N',O']copper(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.067
wR factor = 0.155
Data-to-parameter ratio = 14.3

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

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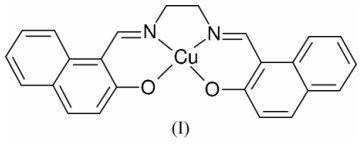
The title complex, [Cu($C_{24}H_{18}N_2O_2$)], has been synthesized and characterized. It is a mononuclear copper(II) complex. The Cu atom is four-coordinated by two N atoms and two O atoms of the bis-Schiff base ligand in a slightly distorted square-planar geometry.

Comment

Transition metal complexes containing Schiff base ligands have been of great interest for many years (Yamada, 1999). These complexes play an important role in the coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures. As an extension of work on the structural characterization of Schiff base complexes, a mononuclear copper(II) complex, (I), is reported here.



(I)

Complex (I) is a mononuclear copper(II) compound (Fig. 1). The central Cu atom is coordinated by two O atoms and two N atoms of the bis-Schiff base ligand. This CuO_2N_2 coordination has a slightly distorted square-planar geometry. The Cu atom is 0.012 (4) Å out of the mean plane of the four donor atoms. The average Cu—O bond length of 1.843 (3) Å (Table 1) is a little shorter than the corresponding value of 1.880 (2) Å observed in a similar Schiff base copper(II) complex (Burgess *et al.*, 2001). The average Cu—N bond distance of 1.833 (3) Å is much shorter than the value of 2.009 (3) Å observed in the same complex. The N—Cu—O *trans* angles are 178.47 (14) and 176.97 (14)°, indicating a slight distortion of the square-planar coordination. Atom C12 deviates from the CuN_2O_2 square plane by 0.125 (6) Å, whereas C13 deviates from it on the opposite side by 0.417 (6) Å. The CuN_2O_2 square plane has dihedral angles of 4.4 (4) and 7.1 (4)° with the two naphthalene ring systems. The dihedral angle between the two naphthalene ring systems is 5.5 (4)°.

Experimental

All chemicals used were commercially available (reagent grade). 2-Hydroxy-1-naphthaldehyde (0.2 mmol, 34.4 mg) and 1,2-diaminoethane (0.1 mmol, 6.0 mg) were dissolved in methanol (10 ml). The mixture was stirred for 1 h to give a clear yellow solution of *L* (0.1 mmol), where *L* is *N*,*N*′-bis(2-hydroxynaphthylmethylidene)-ethane-1,2-diamine. To the solution of *L* was added a methanol

solution (12 ml) of $Cu(CH_3COO)_2{\cdot}H_2O$ (0.1 mmol, 20.0 mg) with stirring. After keeping the resulting solution at room temperature in air for 11 d, blue crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator over anhydrous $CaCl_2$ (yield 61.9%). Analysis found: C 66.8, H 4.3, N 6.4%; calculated for $C_{24}H_{18}CuN_2O_2$: C 67.0, H 4.2, N 6.5%.

Crystal data

$[Cu(C_{24}H_{18}N_2O_2)]$	D_x = 1.558 Mg m^{-3}
M_r = 429.94	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2872 reflections
a = 17.644 (4) Å	θ = 2.7–25.2°
b = 8.165 (2) Å	μ = 1.22 mm^{-1}
c = 12.922 (3) Å	T = 293 (2) K
β = 99.99 (3)°	Block, blue
V = 1833.4 (7) Å^3	0.32 × 0.18 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3743 independent reflections
φ and ω scans	3007 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.038
T_{min} = 0.697, T_{max} = 0.888	θ_{max} = 26.5°
8092 measured reflections	$h = -22 \rightarrow 22$
	$k = -10 \rightarrow 4$
	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.067	$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.155	$(\Delta/\sigma)_{max} < 0.001$
S = 1.15	$\Delta\rho_{max}$ = 0.66 e Å^{-3}
3743 reflections	$\Delta\rho_{min}$ = −0.43 e Å^{-3}
262 parameters	

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.830 (3)	Cu1—O1	1.842 (3)
Cu1—N1	1.837 (3)	Cu1—O2	1.846 (3)
N2—Cu1—N1	86.61 (15)	N2—Cu1—O2	93.18 (14)
N2—Cu1—O1	176.97 (14)	N1—Cu1—O2	178.47 (14)
N1—Cu1—O1	93.60 (14)	O1—Cu1—O2	86.69 (12)

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.96 Å and U_{iso}(H) = 0.08 Å^2.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

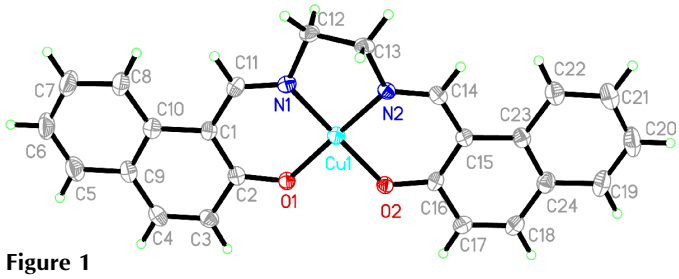


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

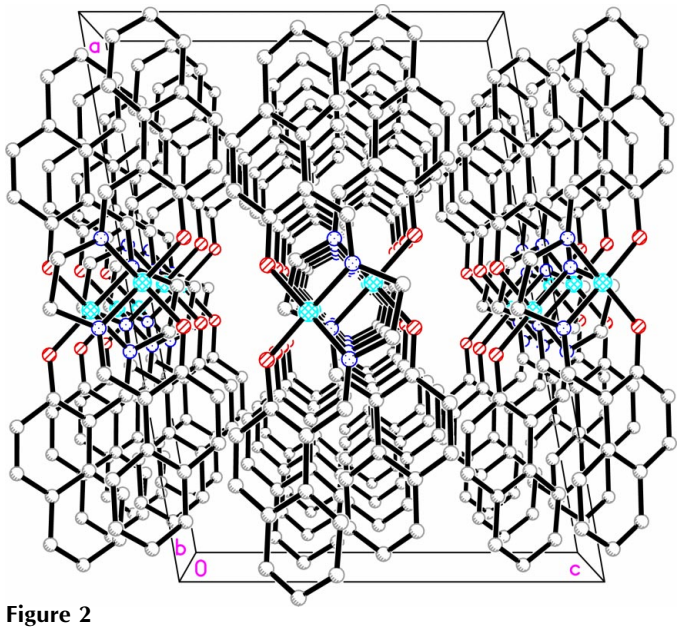


Figure 2
The crystal packing of (I), viewed along the *b* axis.

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