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[*N*,*N*′-Bis(2-oxidobenzylidene)propane-1,3-diamine]copper(II) methanol solvate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
H-atom completeness 81%
Disorder in solvent or counterion
R factor = 0.047
wR factor = 0.134
Data-to-parameter ratio = 16.9

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

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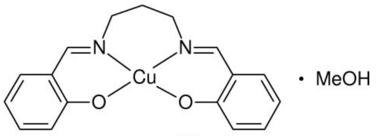
In the electronically neutral complex, $[Cu(C_{17}H_{16}N_2O_2)]\cdot CH_3OH$, the Cu^{II} ion is coordinated by two N atoms and two O atoms from a bis-Schiff base ligand in a slightly distorted square-planar geometry. The methanol solvent molecule is disordered over two orientations.

Comment

The condensation products of 1,3-diaminopropane with salicylaldehyde and its derivatives are present in a large number of transition metal complexes. They may behave as *N*,*O*,*O*′-tridentate anions (Banerjee *et al.*, 2005) or *N*,*N*′,*O*,*O*′-tetradentate dianions (You *et al.*, 2004*a*,*b*,*c*). As part of a study of the structures of these Schiff base compounds, the crystal structure of the title compound, (I), is reported here.



(I)

The title compound is an electronically neutral mononuclear copper(II) complex (Fig. 1). The Cu^{II} ion in the compound is four-coordinated by two O atoms and two N atoms from the Schiff base ligand. This CuO_2N_2 coordination forms a distorted square-planar geometry, as is commonly observed in the structures of Cu^{II}–Schiff base complexes (for example, Han *et al.*, 2001). The dihedral angle between the two benzene rings is 33.4 (3)°.

Experimental

Salicylaldehyde (2.0 mmol, 244 mg) and 1,3-diaminopropane (1.0 mmol, 74 mg) were dissolved in methanol (10 ml). The mixture was stirred for 10 min at 323 K to give a clear yellow solution. A methanol solution (10 ml) of $Cu(NO_2)_2$ (1.0 mmol, 155 mg) was then added. The mixture was stirred for 20 min at room temperature and then filtered. After keeping the filtrate in air for 7 d, black block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent, in about 32% yield. Elemental analysis found: C 57.47, H 5.40, N 7.43%; calculated: C 57.51, H 5.36, N 7.45%.

Crystal data

$[Cu(C_{17}H_{16}N_2O_2)]\cdot CH_4O$
M_r = 375.90
Monoclinic, $P2_1/c$
a = 10.9883 (14) Å
b = 14.7789 (19) Å
c = 10.3156 (13) Å
β = 94.418 (2)°
V = 1670.2 (4) Å^3
Z = 4
D_x = 1.493 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 292 (2) K
Block, black
0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.619$, $T_{\max} = 0.778$
19031 measured reflections
3834 independent reflections
2746 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.103$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.134$
$S = 0.98$
3834 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0785P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.41$ e Å^{-3}
$\Delta\rho_{\min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.914 (2)	Cu1—N1	1.958 (2)
Cu1—O2	1.907 (2)	Cu1—N2	1.972 (3)
O1—Cu1—O2	84.77 (9)	O2—Cu1—N1	156.23 (10)
O1—Cu1—N1	92.01 (9)	O2—Cu1—N2	93.74 (9)
O1—Cu1—N2	159.96 (11)	N1—Cu1—N2	97.05 (10)

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 and 0.97Å, and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The methanol molecule is disordered over two orientations, with C18 common to both. The site-occupancy factors of O3 and O3′ were refined to be 0.713 (6) and 0.287 (6), respectively. The C—O bond lengths were restrained to be 1.385 (10)Å, and all C and O atoms were restrained to approximate isotropic behaviour. H atoms were omitted from the methanol molecule.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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: *SHELXL97*.

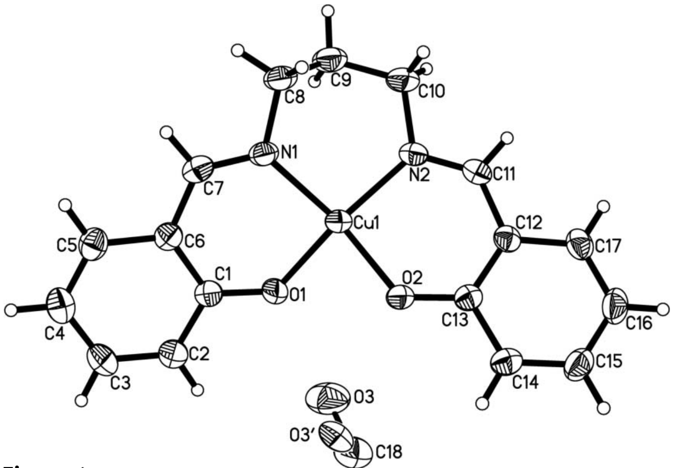


Figure 1
The structure of the title compound, (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probabilty level. H atoms are shown as spheres of arbitrary size.

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