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Azido{1-[(2-diethylaminoethylimino)-methyl]naphthalato}copper(II)

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Key indicators

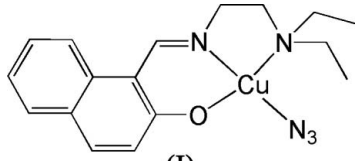
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.055
wR factor = 0.156
Data-to-parameter ratio = 17.6

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

The title compound, $[Cu(C_{17}H_{21}N_2O)(N_3)]$, is a mononuclear copper(II) complex. The central Cu^{II} ion is four-coordinated by one O and two N atoms of the Schiff base ligand, and by one N atom of an azide anion, forming a distorted square-planar coordination geometry.

Comment

Schiff base complexes have been studied extensively, due to their interesting structures and broad applications (Bhaduri *et al.*, 2003; You, 2006*a*,*b*). As an extension of work on the structural characterization of such complexes, a new mononuclear Schiff base copper(II) complex, (I), is reported here.



(I)

The central Cu^{II} cation in compound (I) (Fig. 1) has a distorted square-planar coordination, bonded to one O and two N atoms of a Schiff base ligand, and to one N atom of an azide anion. The bond lengths (Table 1) subtended at the Cu atom are comparable with the corresponding values observed in other Schiff base copper(II) complexes (Mukherjee *et al.*, 2003; Koh *et al.*, 1996).

In the crystal structure, molecules are linked through intermolecuar C—H···N hydrogen bonds (Table 2), forming zigzag chains running along the *b* axis (Fig. 2).

Experimental

2-Hydroxy-1-naphthaldehyde (0.1 mmol, 17.2 mg), *N*,*N*-diethylethane-1,2-diamine (0.1 mmol, 11.6 mg), NaN_3 (0.1 mmol, 6.5 mg) and $Cu(CH_3COO)_2{\cdot}H_2O$ (0.1 mmol, 19.9 mg) were dissolved in methanol (20 ml). The mixture was stirred at room temperature for 1 h to give a clear blue solution. After keeping the solution in air for 8 d, blue block-shaped crystals of (I) were formed.

Crystal data

$[Cu(C_{17}H_{21}N_2O)(N_3)]$
M_r = 374.93
Orthorhombic, *Pbca*
a = 7.195 (1) Å
b = 13.888 (2) Å
c = 33.602 (4) Å
V = 3357.7 (8) Å^3
Z = 8
D_x = 1.483 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 298 (2) K
Block, blue
0.36 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.649, T_{max} = 0.880
26881 measured reflections
3851 independent reflections
2794 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.156
S = 1.03
3851 reflections
219 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0716P)^2 + 4.7533P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.886 (3)	Cu1—N3	1.946 (3)
Cu1—N1	1.912 (3)	Cu1—N2	2.070 (3)
O1—Cu1—N1	93.20 (11)	O1—Cu1—N2	167.42 (13)
O1—Cu1—N3	93.18 (14)	N1—Cu1—N2	84.90 (12)
N1—Cu1—N3	167.61 (18)	N3—Cu1—N2	91.12 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···N3	0.97	2.50	3.066 (5)	117
C14—H14B···N5^{i}	0.97	2.56	3.445 (5)	152

Symmetry code: (i) $-x-\frac{1}{2}, y+\frac{1}{2}, z$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2 or 1.5 timesU_{eq}(C).

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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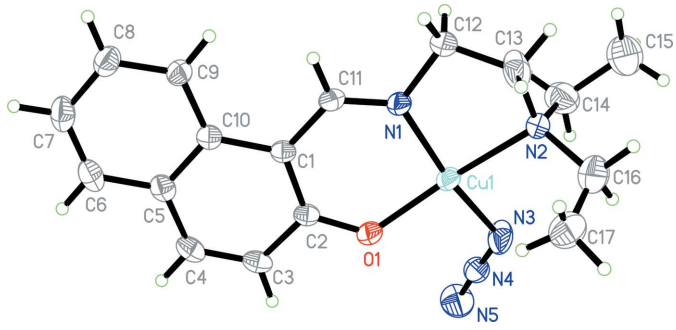

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

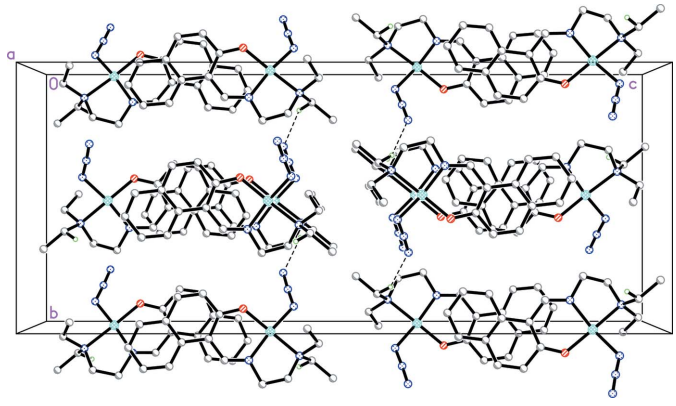

Figure 2
The crystal packing of (I), viewed along the *a* axis. Intermolecular C—H···N hydrogen bonds are shown as dashed lines. H atoms not involved in these hydrogen bonds have been omitted.

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