

Azido{1-[2-(dimethylamino)ethylimino-
methyl]naphthalenolato}copper(II)Qi-Yong Zhu, Yi-Jun Wei* and
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Key indicators

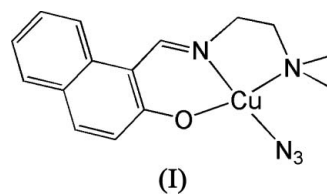
Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.049
 wR factor = 0.139
Data-to-parameter ratio = 17.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title mononuclear copper(II) complex, $[\text{Cu}(\text{C}_{15}\text{H}_{17}\text{N}_2\text{O})\text{N}_3]$, the Cu^{II} ion is four-coordinate in a square-planar geometry defined by the imine and amine N atoms, the naphthalenolate O atom of the Schiff base and a terminal N atom of the azide anion.

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Comment

Schiff base ligands have played an important role in the development of coordination chemistry as they readily form stable complexes with most transition metal ions (Pal *et al.*, 2005; Ueno *et al.*, 2004). During the last few years, there has been a great effort to identify the biological role of copper, primarily through techniques associated with the interface of biology, biochemistry and coordination chemistry (Collinson & Fenton, 1996; Hossain *et al.*, 1996; Tarafder *et al.*, 2002). It appears that the biological role of copper is primarily in redox reactions and as a biological catalyst, although much remains to be understood (Musie *et al.*, 2003; García-Raso *et al.*, 2003). An extensive effort has been made to prepare and characterize a variety of copper(II) coordination complexes in an attempt to model the physical and chemical behaviour of copper-containing enzymes (Reddy *et al.*, 2000). The peculiarity of copper lies in its ability to form complexes with coordination number four, five, and six (Ray *et al.*, 2003; Arnold *et al.*, 2003; Raptopoulou *et al.*, 1998). Recently, we reported a mononuclear copper(II) complex, azido{2,4-dichloro-6-[2-(diethylamino)ethyliminomethyl]phenolato}-copper(II), (II), derived from the Schiff base ligand 2,4-dichloro-6-[2-(diethylamino)ethyliminomethyl]phenol (Wei & Wang, 2006). As an extension of our work on complexes derived from the Schiff bases (Wei, 2005*a,b*), the title copper(II) complex, (I), has been investigated.



The Cu^{II} ion in (I) is four-coordinated by imine and amine N atoms, a naphthalenolate O atom derived from the Schiff base and a terminal N atom of the azide anion, giving a square planar geometry (Fig. 1). The Cu–ligand bond lengths (Table 1) are comparable with the corresponding values observed in (II), and within normal ranges expected for Cu–Schiff base structures (Hebbachi & Benali-Cherif, 2005; Butcher *et al.*, 2003; Elmali *et al.*, 2000; Warda *et al.*, 1997). The bond angles around the central metal in (I) are comparable to

those in (II), and also show some deviations from ideal square-planar geometry (Table 1). In the crystal structure, molecules are linked by weak C12—H12A···O1 hydrogen bonds [C12—H12A = 0.97 Å, H12A···O1ⁱ = 2.56 Å, C12···O1ⁱ = 3.33 Å and C12—H12A···O1ⁱ = 136°; symmetry code: (i) $\frac{1}{2} - x, -\frac{1}{2} + y, z$], forming chains running along the *b* axis (Fig. 2).

Experimental

2-Hydroxy-1-naphthaldehyde (1.0 mmol, 172.2 mg), *N,N*-dimethylethane-1,2-diamine (1.0 mmol, 88.2 mg), NaN₃ (1.0 mmol, 65.3 mg) and Cu(CH₃COO)₂·H₂O (1.0 mmol, 199.1 mg) were dissolved in MeOH (150 ml). The mixture was refluxed at 340 K for about 1 h to give a clear blue solution. After keeping the cooled solution in the dark for 13 d, blue block-shaped crystals of (I) were formed.

Crystal data

[Cu(C ₁₅ H ₁₇ N ₂ O)N ₃]	Mo K α radiation
<i>M_r</i> = 346.88	Cell parameters from 10382 reflections
Orthorhombic, <i>Pbca</i>	θ = 2.6–27.5°
<i>a</i> = 7.568 (1) Å	μ = 1.44 mm ⁻¹
<i>b</i> = 13.306 (1) Å	<i>T</i> = 298 (2) K
<i>c</i> = 30.280 (2) Å	Block, blue
<i>V</i> = 3049.2 (5) Å ³	0.22 × 0.12 × 0.10 mm
<i>Z</i> = 8	
<i>D_x</i> = 1.511 Mg m ⁻³	

Data collection

Bruker SMART CCD area-detector diffractometer	3486 independent reflections
ω scans	2935 reflections with <i>I</i> > 2 σ (<i>I</i>)
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R</i> _{int} = 0.026
<i>T</i> _{min} = 0.742, <i>T</i> _{max} = 0.869	θ _{max} = 27.5°
32372 measured reflections	<i>h</i> = -9 → 9
	<i>k</i> = -17 → 17
	<i>l</i> = -38 → 38

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 3.4391P]$
$R[F^2 > 2\sigma(F^2)] = 0.049$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.139$	(Δ/σ) _{max} < 0.001
<i>S</i> = 1.09	$\Delta\rho_{max} = 1.04 \text{ e \AA}^{-3}$
3486 reflections	$\Delta\rho_{min} = -0.29 \text{ e \AA}^{-3}$
201 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.818 (2)	Cu1—N3	1.904 (3)
Cu1—N1	1.839 (2)	Cu1—N2	1.952 (3)
O1—Cu1—N1	94.05 (10)	O1—Cu1—N2	179.06 (11)
O1—Cu1—N3	89.40 (12)	N1—Cu1—N2	86.80 (12)
N1—Cu1—N3	176.01 (13)	N3—Cu1—N2	89.74 (13)

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with *U*_{iso}(H) = 1.2 or 1.5*U*_{eq}(C). An unassigned maximum residual density peak was observed 1.23 Å from atom C13.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 1997); software used to prepare material for publication: SHELXTL.

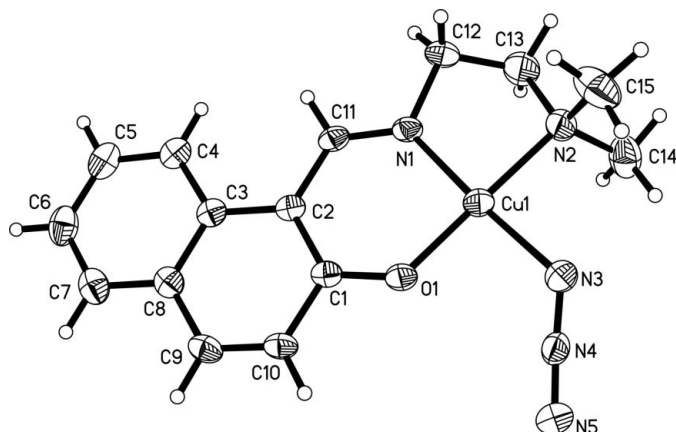


Figure 1

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

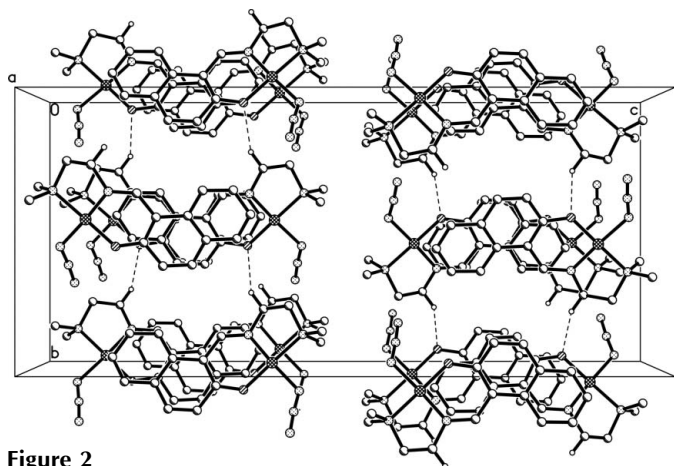


Figure 2

The crystal packing of (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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