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(Nitrato-κO)[1-(pyridin-2-ylmethyliminomethyl)-naphthalen-2-olato-κO]copper(II)

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.101
Data-to-parameter ratio = 14.1

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

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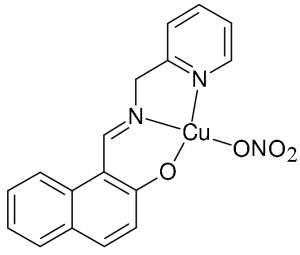
The title compound, $[Cu(C_{17}H_{13}N_3O_4)(NO_3)]$, is a mononuclear copper(II) compound. The Cu atom is coordinated by two N atoms and one O atom from the Schiff base ligand, and by one O atom from a nitrate anion. The four atoms around the metal adopt a slightly distorted square-planar geometry.

Comment

Recently, we have reported a few Schiff base complexes (You, Lin *et al.*, 2003; You, Qu *et al.*, 2003; You, Xiong *et al.*, 2004; You, Zhu & Liu, 2004). As an extension of our work on the structural characterization of Schiff base complexes, the title mononuclear copper(II) complex, (I), is reported here.



(I)

The structure of (I) (Fig. 1) contains a mononuclear copper(II) complex. The Cu atom is in a square-planar geometry and is four-coordinated by one O and two N atoms from the Schiff base ligand, and by one O atom from the coordinated nitrate anion. The four coordinating atoms around the Cu centre are approximately coplanar, giving a square-planar geometry with an average deviation of 0.006 (3) Å; the Cu atom lies 0.036 (2) Å above this plane.

The C11═N2 bond distance [1.287 (3) Å; Table 1] conforms to the value for a double bond, while the C12—N2 bond

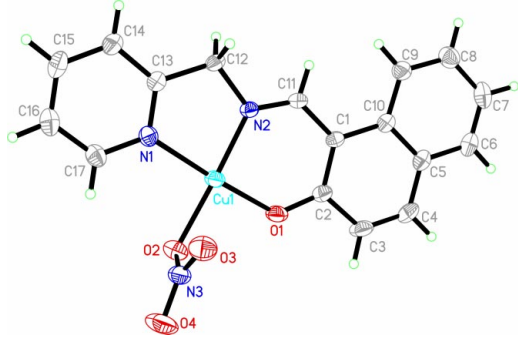


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

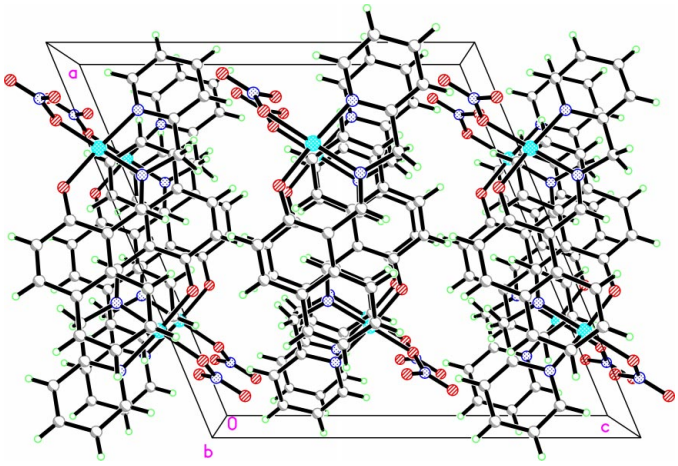


Figure 2
Crystal packing of (I), viewed along the *b* axis.

distance [1.465 (3) Å] conforms to the value for a single bond. The Cu1—O1 bond length [1.875 (2) Å] is a little shorter than the value [1.889 (2) Å] observed in another Schiff base complex (You, Chen *et al.*, 2004). The Cu1—N2 bond distance [1.916 (2) Å] is also a little shorter than the value [1.927 (3) Å] observed in the same complex. The Cu1—N1 and Cu1—O2 distances are also comparable to the values found in most copper(II) complexes (Butcher *et al.*, 2003). The bond angles around the Cu^{II} centre show some deviations from ideal square-planar geometry.

Experimental

All chemicals used (reagent grade) were commercially available. 2-Hydroxy-1-naphthaldehyde (0.1 mmol, 17.2 mg) and 2-aminomethylpyridine (0.1 mmol, 10.8 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 1 h to give a clear yellow solution of HL, where H*L* is 1-(pyridin-2-ylmethyliminomethyl)naphthalen-2-ol. To the solution of H*L* was added a methanol solution (10 ml) of $Cu(NO_3)_2{\cdot}4H_2O$ (0.1 mmol, 26.0 mg), with stirring. The mixture was stirred for another 1 h at room temperature and then filtered. After keeping the filtrate in air for 8 d, blue block-shaped 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 using anhydrous $CaCl_2$ (yield 69.3%). Analysis found: C 52.6, H 3.6, N 10.7%; calculated for $C_{17}H_{13}CuN_3O_4$: C 52.8, H 3.4, N 10.9%.

Crystal data

$[Cu(C_{17}H_{13}N_3O_4)(NO_3)]$	D_x = 1.658 Mg m^{-3}
M_r = 386.84	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2267 reflections
a = 15.093 (3) Å	θ = 2.7–25.2°
b = 7.394 (2) Å	μ = 1.44 mm^{-1}
c = 15.062 (3) Å	T = 273 (2) K
β = 112.766 (3)°	Block, blue
V = 1550.0 (6) Å^3	0.32 × 0.28 × 0.23 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3176 independent reflections
φ and ω scans	2523 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.031
T_{min} = 0.656, T_{max} = 0.733	θ_{max} = 26.5°
8707 measured reflections	$h = -18 \rightarrow 15$
	$k = -9 \rightarrow 9$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.2644P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.101	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
3176 reflections	
226 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.875 (2)	Cu1—N1	1.979 (2)
Cu1—N2	1.916 (2)	Cu1—O2	2.011 (2)
O1—Cu1—N2	93.07 (8)	O1—Cu1—O2	88.59 (8)
O1—Cu1—N1	176.24 (8)	N2—Cu1—O2	177.02 (9)
N2—Cu1—N1	83.60 (9)	N1—Cu1—O2	94.65 (9)

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) = 1.2U_{eq}(C).

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*.

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References

Butcher, R. J., Mockler, G. M. & McKern, O. (2003). *Acta Cryst.* E**59**, m1104–m1106.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
You, Z.-L., Chen, B., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst.* E**60**, m884–m886.
You, Z.-L., Lin, Y.-S., Tan, M.-Y. & Zhu, H.-L. (2003). *Acta Cryst.* E**59**, m1025–m1027.
You, Z.-L., Qu, Y., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2003). *Acta Cryst.* E**59**, m1038–m1040.
You, Z.-L., Xiong, Z.-D., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, m79–m81.
You, Z.-L., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst.* E**60**, m560–m562.