

**(2,2'-Bipyridine- $\kappa^2N,N'$ )[*N*-(2-oxido-1-naphthylidene)threoninato- $\kappa^3O^1,N,O^2$ ]-copper(II)**

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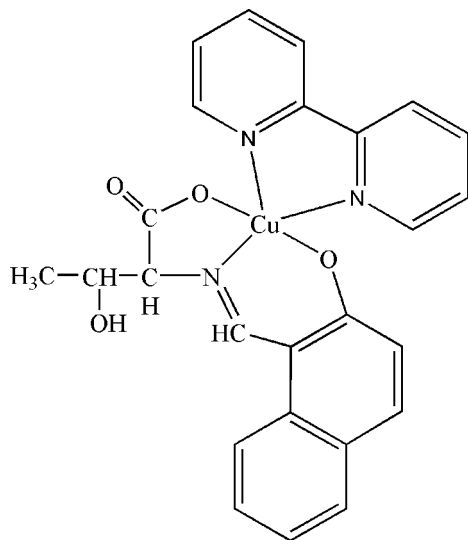
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(C-C) = 0.005$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.089; data-to-parameter ratio = 17.6.

In the title complex,  $[Cu(C_{15}H_{13}NO_4)(C_{10}H_8N_2)]$ , the Schiff base ligand is derived from the condensation of 2-hydroxy-1-naphthaldehyde and L-threonine. The  $Cu^{II}$  atom is five-coordinated by one N atom and two O atoms from the Schiff base ligand and by two N atoms from a 2,2'-bipyridine ligand in a distorted square-pyramidal geometry. In the crystal structure, the combination of intermolecular  $O-H\cdots O$  and  $C-H\cdots O$  hydrogen bonds leads to a two-dimensional network.

**Related literature**

For related literature, see: Garnovski *et al.* (1993); Kalagouda *et al.* (2006); Wang *et al.* (1999).

**Experimental***Crystal data*

$[Cu(C_{15}H_{13}NO_4)(C_{10}H_8N_2)]$   
 $M_r = 490.99$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 9.955$  (2) Å  
 $b = 12.180$  (3) Å  
 $c = 18.438$  (4) Å

$V = 2235.6$  (9) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.01$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 $0.29 \times 0.28 \times 0.16$  mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.757$ ,  $T_{max} = 0.855$

14242 measured reflections  
 5278 independent reflections  
 4243 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.027$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.088$   
 $S = 1.04$   
 5278 reflections  
 300 parameters  
 492 restraints

H-atom parameters constrained  
 $\Delta\rho_{max} = 0.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.54$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), 2229 Friedel pairs  
 Flack parameter:  $-0.005$  (13)

**Table 1**

Selected geometric parameters (Å, °).

Cu1—O4	1.925 (2)	Cu1—O1	2.0236 (18)
Cu1—N1	1.926 (2)	Cu1—N2	2.231 (3)
Cu1—N3	2.005 (2)		
O4—Cu1—N1	92.62 (8)	N3—Cu1—O1	92.57 (9)
O4—Cu1—N3	91.77 (9)	O4—Cu1—N2	109.51 (10)
N1—Cu1—N3	174.65 (9)	N1—Cu1—N2	104.07 (9)
O4—Cu1—O1	147.49 (9)	N3—Cu1—N2	77.29 (10)
N1—Cu1—O1	82.08 (8)	O1—Cu1—N2	102.88 (9)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 <sup>i</sup> ···O2 <sup>i</sup>	0.82	1.99	2.808 (3)	178
C5—H11 <sup>i</sup> ···O2 <sup>i</sup>	0.93	2.49	3.311 (3)	147
C12—H27 <sup>i</sup> ···O2 <sup>i</sup>	0.93	2.50	3.431 (4)	174
C14—H25 <sup>ii</sup> ···O3 <sup>ii</sup>	0.93	2.52	3.445 (4)	177

Symmetry codes: (i)  $x - \frac{1}{2}, -y + \frac{5}{2}, -z + 2$ ; (ii)  $-x - \frac{1}{2}, -y + 2, z - \frac{1}{2}$ .

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2129).

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**supplementary materials**

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**(2,2'-Bipyridine- $\kappa^2N,N'$ )[*N*-(2-oxido-1-naphthylidene)threoninato- $\kappa^3O^1,N,O^2$ ]copper(II)**

**Z. Qiu, L. Li, Y. Liu, T. Xu and D. Wang**

**Comment**

Amino acids and their derivatives are very important in molecular biology because of their roles in biochemical reactions. Schiff base complexes have continued to play the role of the most important stereochemical models in main group and transition metal coordination chemistry with their easy preparation and structural variation (Garnovski *et al.*, 1993). So efforts have been made to synthesize and characterize amino Schiff base complexes with transition metals and more and more these new complexes have been reported (Kalagouda *et al.*, 2006; Wang *et al.*, 1999). Herein, we report the synthesis and crystal structure of a copper(II) complex with a tridentate Schiff base ligand derived from the condensation of 2-hydroxy-1-naphthaldehyde and L-threonine.

In the title compound (Fig. 1), the Cu<sup>II</sup> atom is in a distorted square-pyramidal coordination geometry, defined by one N and two O atoms from the Schiff base ligand and two N atoms from a 2, 2'-bipyridine ligand. The Cu atom deviates from the basal equatorial plane (formed by O1, N1, O4 and N3) by 0.230 (2) Å toward N2 atom, with a significantly longer Cu1—N2 bond distance (Table 1). The Cu1—N2 bond deviates greatly from the right position to close the Cu1—N3 bond [the bond angle of N3—Cu1—N2 is 77.3 (1)°]. The bipyridine ligand deviates from planarity, with an angle of 11.7 (1)° between the two pyridyl rings. The least-square plane of the bipyridine ligand is approximately perpendicular to the basal equatorial plane [dihedral angle 100.3 (2)°]. In the crystal, the combination of intermolecular O—H···O and C—H···O hydrogen bonds (Table 2) leads to a two-dimensional network structure (Fig. 2).

**Experimental**

L-Threonine (0.119 g, 1 mmol) was dissolved in hot methanol (10 ml), which was then added to a methanol solution (3 ml) of 2-hydroxy-1-naphthaldehyde (0.172 g, 1 mmol). The mixture was stirred at 323 K for 2 h. Subsequently, an aqueous solution (2 ml) of cupric acetate monohydrate (0.200 g, 1 mmol) was added dropwise and stirred for 2 h. A methanol solution (5 ml) of 2,2'-bipyridine (0.156 g, 1 mmol) was added dropwise and stirred for 4 h. The solution was held at room temperature for 10 d and blue block crystals suitable for X-ray diffraction were obtained.

**Refinement**

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.98(CH) and 0.96(CH<sub>3</sub>) Å, and O—H = 0.82 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{C},\text{O})$  for methyl and hydroxyl groups.

## Figures

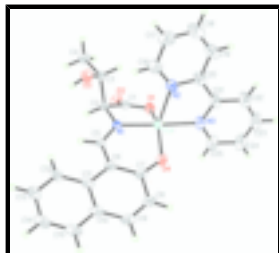


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

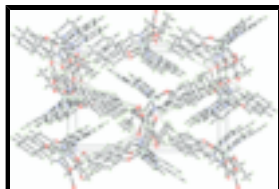


Fig. 2. Packing diagram of the title compound with hydrogen bonds shown as dashed lines.

## (2,2'-Bipyridine- $\kappa^2N,N'$ )[N-(2-oxido-1-naphthylidene)threoninato- $\kappa^3O^1,N,O^2$ ]copper(II)

### Crystal data

[Cu(C<sub>15</sub>H<sub>13</sub>NO<sub>4</sub>)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)]

$M_r = 490.99$

Orthorhombic,  $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 9.955 (2) \text{ \AA}$

$b = 12.180 (3) \text{ \AA}$

$c = 18.438 (4) \text{ \AA}$

$V = 2235.6 (9) \text{ \AA}^3$

$Z = 4$

$F_{000} = 1012$

$D_x = 1.459 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 5604 reflections

$\theta = 2.3\text{--}26.1^\circ$

$\mu = 1.01 \text{ mm}^{-1}$

$T = 298 (2) \text{ K}$

Block, blue

$0.29 \times 0.28 \times 0.16 \text{ mm}$

### Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2) \text{ K}$

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.757$ ,  $T_{\max} = 0.855$

14242 measured reflections

5278 independent reflections

4243 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 28.3^\circ$

$\theta_{\min} = 2.0^\circ$

$h = -13 \rightarrow 13$

$k = -14 \rightarrow 16$

$l = -20 \rightarrow 24$

Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2]$
$wR(F^2) = 0.089$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{\max} = 0.001$
5278 reflections	$\Delta\rho_{\max} = 0.32 \text{ e } \text{\AA}^{-3}$
300 parameters	$\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$
492 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2229 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: $-0.005 (13)$

Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.32501 (3)	1.00767 (2)	0.977106 (17)	0.03806 (10)
N1	0.1622 (2)	1.08781 (15)	0.95744 (11)	0.0313 (4)
N2	0.2672 (3)	0.89079 (19)	1.06492 (15)	0.0491 (6)
N3	0.5005 (2)	0.93672 (19)	1.00252 (14)	0.0480 (6)
O4	0.3191 (2)	0.93362 (17)	0.88490 (11)	0.0498 (5)
O2	0.29386 (19)	1.31490 (16)	1.05070 (12)	0.0512 (5)
O1	0.37076 (18)	1.14608 (15)	1.03256 (11)	0.0424 (4)
O3	-0.05190 (19)	1.07490 (16)	1.05400 (12)	0.0474 (5)
H3	-0.0961	1.1082	1.0236	0.071*
C1	0.2783 (3)	1.2178 (2)	1.03223 (14)	0.0371 (6)
C2	0.1394 (3)	1.17825 (19)	1.00763 (13)	0.0319 (5)
H28	0.0912	1.2379	0.9832	0.038*
C3	0.0596 (3)	1.1395 (2)	1.07501 (15)	0.0368 (6)
H29	0.1194	1.0925	1.1037	0.044*
C4	0.0177 (3)	1.2351 (3)	1.12313 (16)	0.0510 (7)
H21A	-0.0285	1.2076	1.1651	0.077*
H21B	-0.0409	1.2830	1.0965	0.077*
H21C	0.0960	1.2750	1.1382	0.077*
C5	0.0856 (2)	1.0765 (2)	0.90139 (14)	0.0325 (5)
H11	0.0125	1.1237	0.8978	0.039*
C6	0.1028 (2)	0.9982 (2)	0.84450 (12)	0.0363 (5)

## supplementary materials

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C7	0.2228 (3)	0.9366 (2)	0.83774 (15)	0.0415 (6)
C8	0.2402 (3)	0.8722 (3)	0.77391 (16)	0.0545 (8)
H18	0.3199	0.8335	0.7678	0.065*
C9	0.1453 (4)	0.8654 (3)	0.72205 (16)	0.0560 (8)
H19	0.1615	0.8224	0.6813	0.067*
C10	0.0215 (3)	0.9221 (2)	0.72803 (15)	0.0452 (6)
C11	-0.0016 (3)	0.9893 (2)	0.78988 (13)	0.0397 (6)
C12	-0.1269 (3)	1.0408 (2)	0.79527 (17)	0.0495 (7)
H27	-0.1453	1.0845	0.8354	0.059*
C13	-0.2234 (4)	1.0284 (3)	0.74247 (19)	0.0588 (8)
H26	-0.3055	1.0640	0.7475	0.071*
C14	-0.2000 (4)	0.9635 (3)	0.68174 (18)	0.0621 (9)
H25	-0.2659	0.9556	0.6464	0.074*
C15	-0.0795 (4)	0.9115 (3)	0.67446 (17)	0.0572 (8)
H15	-0.0634	0.8685	0.6337	0.069*
C16	0.1466 (4)	0.8711 (3)	1.0941 (2)	0.0660 (9)
H17	0.0701	0.8976	1.0710	0.079*
C17	0.1333 (6)	0.8119 (3)	1.1577 (3)	0.0965 (13)
H22	0.0488	0.7999	1.1777	0.116*
C18	0.2463 (6)	0.7710 (4)	1.1912 (3)	0.1063 (14)
H36	0.2387	0.7302	1.2336	0.128*
C19	0.3693 (5)	0.7909 (3)	1.1617 (3)	0.0883 (12)
H37	0.4468	0.7665	1.1849	0.106*
C20	0.3776 (4)	0.8483 (2)	1.09632 (19)	0.0579 (8)
C21	0.5052 (3)	0.8664 (2)	1.05811 (19)	0.0524 (7)
C22	0.6242 (4)	0.8126 (3)	1.0751 (2)	0.0701 (10)
H33	0.6271	0.7624	1.1131	0.084*
C23	0.7371 (4)	0.8343 (3)	1.0354 (3)	0.0775 (11)
H23	0.8169	0.7986	1.0468	0.093*
C24	0.7348 (3)	0.9067 (3)	0.9799 (3)	0.0719 (10)
H24	0.8118	0.9222	0.9532	0.086*
C25	0.6136 (3)	0.9570 (3)	0.9642 (2)	0.0634 (9)
H32	0.6097	1.0066	0.9259	0.076*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.03383 (16)	0.04027 (16)	0.04008 (17)	0.00393 (14)	-0.00421 (14)	0.00230 (15)
N1	0.0301 (10)	0.0347 (10)	0.0291 (11)	0.0002 (9)	0.0011 (9)	-0.0009 (8)
N2	0.0536 (15)	0.0405 (13)	0.0531 (16)	-0.0017 (11)	-0.0030 (13)	0.0083 (12)
N3	0.0409 (13)	0.0384 (13)	0.0647 (17)	0.0035 (10)	-0.0093 (12)	0.0003 (11)
O4	0.0456 (11)	0.0590 (12)	0.0448 (12)	0.0165 (10)	-0.0016 (11)	-0.0084 (9)
O2	0.0434 (11)	0.0466 (11)	0.0636 (14)	-0.0096 (9)	0.0033 (10)	-0.0158 (10)
O1	0.0341 (9)	0.0460 (10)	0.0470 (12)	-0.0025 (8)	-0.0092 (9)	-0.0015 (9)
O3	0.0356 (10)	0.0553 (12)	0.0514 (13)	-0.0103 (9)	0.0020 (9)	0.0047 (10)
C1	0.0398 (13)	0.0424 (13)	0.0291 (13)	-0.0075 (11)	0.0053 (11)	-0.0008 (11)
C2	0.0348 (12)	0.0333 (12)	0.0275 (12)	0.0016 (10)	-0.0021 (10)	-0.0008 (9)
C3	0.0339 (13)	0.0442 (14)	0.0323 (13)	-0.0029 (11)	0.0013 (11)	0.0017 (11)

C4	0.0536 (18)	0.0621 (19)	0.0374 (15)	0.0016 (15)	0.0060 (14)	-0.0050 (14)
C5	0.0326 (12)	0.0360 (12)	0.0288 (12)	0.0016 (10)	-0.0001 (10)	0.0002 (10)
C6	0.0456 (13)	0.0364 (12)	0.0270 (11)	0.0003 (13)	0.0012 (10)	-0.0009 (11)
C7	0.0486 (15)	0.0413 (14)	0.0346 (14)	0.0009 (12)	0.0065 (12)	-0.0036 (11)
C8	0.0637 (19)	0.0570 (17)	0.0428 (17)	0.0105 (15)	0.0104 (15)	-0.0090 (14)
C9	0.074 (2)	0.0580 (16)	0.0354 (15)	-0.0053 (16)	0.0078 (15)	-0.0131 (13)
C10	0.0586 (16)	0.0469 (15)	0.0299 (13)	-0.0123 (13)	0.0007 (13)	-0.0025 (11)
C11	0.0510 (14)	0.0392 (13)	0.0291 (11)	-0.0082 (13)	-0.0017 (11)	0.0002 (11)
C12	0.0552 (16)	0.0542 (15)	0.0392 (15)	-0.0003 (13)	-0.0115 (13)	-0.0065 (12)
C13	0.0596 (17)	0.065 (2)	0.0515 (17)	-0.0031 (15)	-0.0187 (15)	-0.0011 (15)
C14	0.076 (2)	0.0662 (18)	0.0440 (16)	-0.0210 (16)	-0.0221 (16)	0.0030 (14)
C15	0.079 (2)	0.0582 (17)	0.0344 (15)	-0.0206 (16)	-0.0067 (15)	-0.0039 (13)
C16	0.074 (2)	0.0503 (17)	0.074 (2)	-0.0007 (16)	0.0131 (19)	0.0167 (16)
C17	0.104 (3)	0.085 (3)	0.101 (3)	0.002 (2)	0.034 (3)	0.038 (2)
C18	0.128 (3)	0.098 (3)	0.092 (3)	0.009 (3)	0.010 (3)	0.049 (2)
C19	0.100 (3)	0.080 (2)	0.084 (2)	0.015 (2)	-0.007 (2)	0.035 (2)
C20	0.0753 (19)	0.0387 (14)	0.0597 (18)	0.0037 (15)	-0.0113 (17)	0.0086 (14)
C21	0.0575 (17)	0.0352 (14)	0.0645 (18)	0.0071 (13)	-0.0215 (15)	-0.0033 (14)
C22	0.076 (2)	0.0502 (17)	0.084 (2)	0.0146 (17)	-0.029 (2)	-0.0012 (17)
C23	0.060 (2)	0.063 (2)	0.109 (3)	0.0182 (17)	-0.031 (2)	-0.020 (2)
C24	0.0489 (17)	0.0566 (18)	0.110 (3)	0.0058 (15)	-0.010 (2)	-0.015 (2)
C25	0.0492 (17)	0.0481 (16)	0.093 (2)	0.0030 (13)	-0.0050 (18)	-0.0026 (16)

*Geometric parameters (Å, °)*

Cu1—O4	1.925 (2)	C8—H18	0.9300
Cu1—N1	1.926 (2)	C9—C10	1.417 (5)
Cu1—N3	2.005 (2)	C9—H19	0.9300
Cu1—O1	2.0236 (18)	C10—C15	1.415 (4)
Cu1—N2	2.231 (3)	C10—C11	1.422 (4)
N1—C5	1.292 (3)	C11—C12	1.400 (4)
N1—C2	1.457 (3)	C12—C13	1.376 (4)
N2—C16	1.338 (4)	C12—H27	0.9300
N2—C20	1.345 (4)	C13—C14	1.390 (5)
N3—C21	1.337 (4)	C13—H26	0.9300
N3—C25	1.352 (4)	C14—C15	1.363 (5)
O4—C7	1.295 (4)	C14—H25	0.9300
O2—C1	1.240 (3)	C15—H15	0.9300
O1—C1	1.269 (3)	C16—C17	1.384 (5)
O3—C3	1.415 (3)	C16—H17	0.9300
O3—H3	0.8200	C17—C18	1.376 (7)
C1—C2	1.533 (4)	C17—H22	0.9300
C2—C3	1.548 (4)	C18—C19	1.362 (7)
C2—H28	0.9800	C18—H36	0.9300
C3—C4	1.522 (4)	C19—C20	1.397 (5)
C3—H29	0.9800	C19—H37	0.9300
C4—H21A	0.9600	C20—C21	1.469 (5)
C4—H21B	0.9600	C21—C22	1.390 (5)
C4—H21C	0.9600	C22—C23	1.366 (6)



## supplementary materials

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C5—C6	1.428 (3)	C22—H33	0.9300
C5—H11	0.9300	C23—C24	1.352 (6)
C6—C7	1.417 (4)	C23—H23	0.9300
C6—C11	1.452 (3)	C24—C25	1.384 (5)
C7—C8	1.425 (4)	C24—H24	0.9300
C8—C9	1.346 (5)	C25—H32	0.9300
O4—Cu1—N1	92.62 (8)	C9—C8—H18	118.8
O4—Cu1—N3	91.77 (9)	C7—C8—H18	118.8
N1—Cu1—N3	174.65 (9)	C8—C9—C10	121.6 (3)
O4—Cu1—O1	147.49 (9)	C8—C9—H19	119.2
N1—Cu1—O1	82.08 (8)	C10—C9—H19	119.2
N3—Cu1—O1	92.57 (9)	C15—C10—C9	121.3 (3)
O4—Cu1—N2	109.51 (10)	C15—C10—C11	119.8 (3)
N1—Cu1—N2	104.07 (9)	C9—C10—C11	118.9 (3)
N3—Cu1—N2	77.29 (10)	C12—C11—C10	117.3 (3)
O1—Cu1—N2	102.88 (9)	C12—C11—C6	123.7 (2)
C5—N1—C2	119.8 (2)	C10—C11—C6	118.9 (3)
C5—N1—Cu1	126.40 (17)	C13—C12—C11	121.5 (3)
C2—N1—Cu1	113.27 (15)	C13—C12—H27	119.3
C16—N2—C20	119.4 (3)	C11—C12—H27	119.3
C16—N2—Cu1	129.6 (2)	C12—C13—C14	121.0 (3)
C20—N2—Cu1	110.3 (2)	C12—C13—H26	119.5
C21—N3—C25	119.3 (3)	C14—C13—H26	119.5
C21—N3—Cu1	119.1 (2)	C15—C14—C13	119.4 (3)
C25—N3—Cu1	121.6 (2)	C15—C14—H25	120.3
C7—O4—Cu1	127.02 (18)	C13—C14—H25	120.3
C1—O1—Cu1	114.08 (16)	C14—C15—C10	120.9 (3)
C3—O3—H3	109.5	C14—C15—H15	119.5
O2—C1—O1	124.4 (2)	C10—C15—H15	119.5
O2—C1—C2	119.6 (2)	N2—C16—C17	121.3 (4)
O1—C1—C2	116.1 (2)	N2—C16—H17	119.3
N1—C2—C1	106.54 (19)	C17—C16—H17	119.3
N1—C2—C3	111.06 (19)	C18—C17—C16	119.4 (5)
C1—C2—C3	108.7 (2)	C18—C17—H22	120.3
N1—C2—H28	110.1	C16—C17—H22	120.3
C1—C2—H28	110.1	C19—C18—C17	119.5 (4)
C3—C2—H28	110.1	C19—C18—H36	120.3
O3—C3—C4	111.7 (2)	C17—C18—H36	120.3
O3—C3—C2	110.6 (2)	C18—C19—C20	119.1 (4)
C4—C3—C2	112.0 (2)	C18—C19—H37	120.4
O3—C3—H29	107.4	C20—C19—H37	120.4
C4—C3—H29	107.4	N2—C20—C19	121.1 (4)
C2—C3—H29	107.4	N2—C20—C21	116.2 (3)
C3—C4—H21A	109.5	C19—C20—C21	122.7 (4)
C3—C4—H21B	109.5	N3—C21—C22	120.3 (4)
H21A—C4—H21B	109.5	N3—C21—C20	115.7 (3)
C3—C4—H21C	109.5	C22—C21—C20	123.9 (3)
H21A—C4—H21C	109.5	C23—C22—C21	119.3 (4)
H21B—C4—H21C	109.5	C23—C22—H33	120.4

N1—C5—C6	126.0 (2)	C21—C22—H33	120.4
N1—C5—H11	117.0	C24—C23—C22	121.2 (3)
C6—C5—H11	117.0	C24—C23—H23	119.4
C7—C6—C5	121.3 (2)	C22—C23—H23	119.4
C7—C6—C11	120.2 (2)	C23—C24—C25	117.5 (4)
C5—C6—C11	118.3 (2)	C23—C24—H24	121.3
O4—C7—C6	125.5 (2)	C25—C24—H24	121.3
O4—C7—C8	116.7 (3)	N3—C25—C24	122.4 (4)
C6—C7—C8	117.8 (3)	N3—C25—H32	118.8
C9—C8—C7	122.4 (3)	C24—C25—H32	118.8
C1—C2—C3—C4	71.0 (3)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O3—H3 $\cdots$ O2 <sup>i</sup>	0.82	1.99	2.808 (3)	178
C5—H11 $\cdots$ O2 <sup>i</sup>	0.93	2.49	3.311 (3)	147
C12—H27 $\cdots$ O2 <sup>i</sup>	0.93	2.50	3.431 (4)	174
C14—H25 $\cdots$ O3 <sup>ii</sup>	0.93	2.52	3.445 (4)	177

Symmetry codes: (i)  $x-1/2, -y+5/2, -z+2$ ; (ii)  $-x-1/2, -y+2, z-1/2$ .

Fig. 1

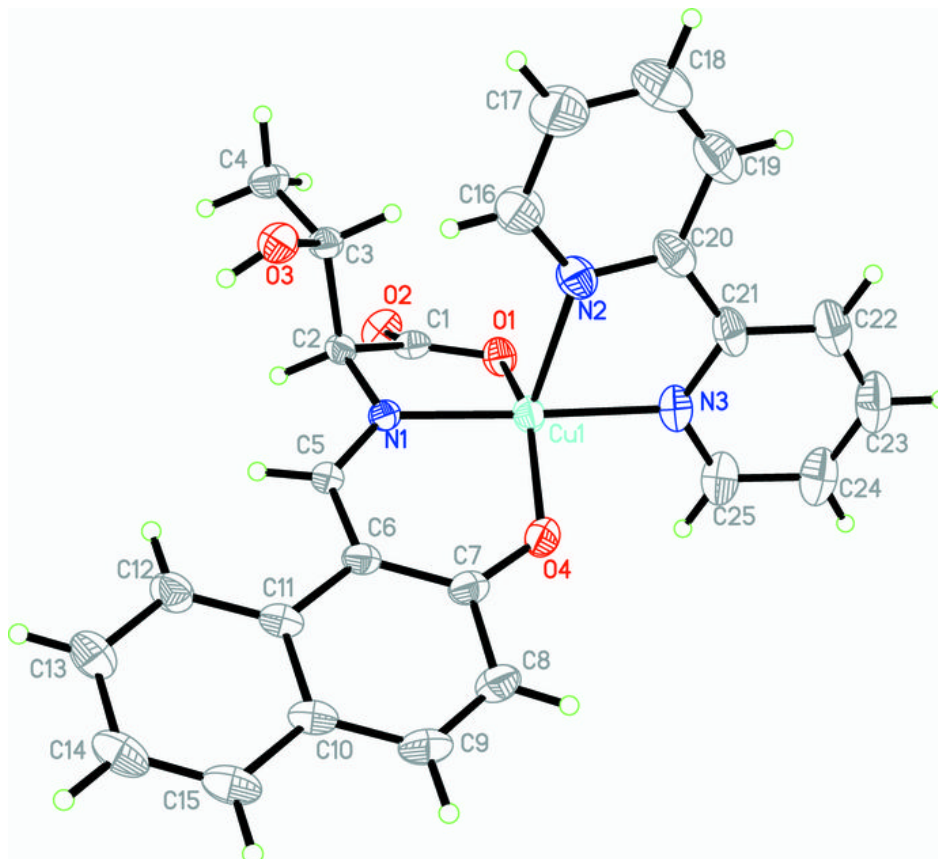


Fig. 2

