Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[2-(3-Methoxy-2-oxidobenzylideneamino)phenolato-κ^3O,N,O'](1,10-phenanthroline-κ^2N,N')copper(II) methanol solvate

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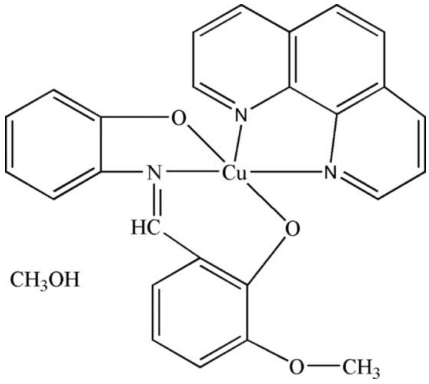
Received 14 April 2007; accepted 26 April 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.040; wR factor = 0.096; data-to-parameter ratio = 12.3.

In the title complex, $[Cu(C_{14}H_{11}NO_3)(C_{12}H_8N_2)]\cdot CH_3OH$, with a tridentate Schiff base ligand derived from the condensation of *o*-vanillin and 2-hydroxyaniline, the Cu^{II} ion is five-coordinated by three N atoms [Cu—N = 1.950 (2)–2.333 (3) Å] and two O atoms [Cu—O = 1.926 (2) and 1.949 (2) Å] in a distorted square-pyramidal configuration. The mean planes of the tridentate Schiff base and 1,10-phenanthroline (phen) ligands make a dihedral angle of 88.39 (5)°. Two neighbouring complexes related by a centre of symmetry are paired by a significant π–π interaction, with a short distance of 3.396 (4) Å between the centroids of the outer rings of the phen ligands. The crystal packing is further stabilized by intermolecular O—H···O and C—H···O hydrogen bonds.

Related literature

For related literature, see: Elena *et al.* (1995).



Experimental

Crystal data

$[Cu(C_{14}H_{11}NO_3)(C_{12}H_8N_2)]\cdot CH_4O$
M_r = 517.02
Triclinic, $P\overline{1}$
a = 9.905 (3) Å
b = 10.335 (3) Å
c = 12.094 (3) Å
α = 82.701 (3)°
β = 70.742 (3)°
γ = 89.236 (3)°
V = 1158.8 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 298 (2) K
0.21 × 0.18 × 0.07 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SABADS*; Sheldrick, 1996)
T_{min} = 0.820, T_{max} = 0.934
5996 measured reflections
4012 independent reflections
3134 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.096
S = 1.03
4012 reflections
325 parameters
16 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3^{i}	0.82	1.93	2.719 (5)	160
O4′—H4′···O3^{i}	0.82	1.92	2.735 (6)	171
C17—H17···O2^{ii}	0.93	2.43	3.204 (4)	141

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

We thank the Natural Science Foundation of Shandong Province for research grant No. Y2004B02.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2231).

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  doi:10.1107/S1600536807020867

supplementary materials

Acta Cryst. (2007). E**63**, m1578 [**doi:10.1107/S1600536807020867**]

[2-(3-Methoxy-2-oxidobenzylideneamino)phenolato-κ^3O,N,O'](1,10-phenanthroline-κ^2N,N')copper(II) methanol solvate

J.-F. Dong, L.-Z. Li, Z.-Z. Ji, H. Cui and D.-Q. Wang

Comment

Schiff bases still play an important role as ligands in metal coordination chemistry since their discovery [Yamada, S. (1966) Coord. Chem. Rew. 1, 415–437]. Considerable efforts have been devotedd to copper(II) complexes of tridentate Schiff base ligands of *N*-alkylidene or *N*-arylidene alkanato type due to their structural richness and a potential model for a number of important biological systems. We report here the synthesis and crystal structure of the title compound, (I), a new copper(II) complex with a tridentate Schiff base ligand derived from the condensation of *o*-vanillin and 2-Hydroxyaniline, and with phenanthroline.

The Cu^{II} atom is five-coordinataed in a seriously distorted square-pyramidal geometry (Fig.1), in which O1, O3, N1, and N2 locate in equatorial plane, and N3 in the apical position, and the Cu^{II} atom lies 0.1205 (12) Å above the equatorial plane. The bond distances of Cu—N2, Cu—N3 from neutral ligand phenanthroline are somewhat longer than those of Cu—N1, Cu—O1 and Cu—O2 from Schiff base anion(Table 1), similar to that reported previously (Elena *et al.*, 1995). The apical Cu—N3 bond deviates greatly from the right position to close the Cu—N2 bond (N3—Cu1—N2 is 76.37 (9)°). The tridentate Schiff base ligand coordinated to copper atom to form two chelated rings (Cu1/O3/C9—C10/N1 and Cu1/N1/C1—C3/O1) and the two rings has dihedral angle 4.48 (34)° and 2.92 (13)° to the equatorial plane, respectively. The phenanthroline ligand almost perpendicular to the Schiff base chelating plane (dihedral angle 87.96 (7)°). As shown in Fig. 2, the ligands of 1,10-phenanthroline moiety related by centers of symmetry have a centroid-centroid separation of 3.396 (4)Å (perpendicular distance 3.282 (4) Å) for rings formed by C15—C19/N2 atoms and the slip angle is 14.89 (50)°, indicating a significant π-π interaction [Tong, *M. L.*, Lee, H. K., Chen, *X. M.*, Huang, *R.* B., Mak, T. M·C. (1999) J. Chem. Soc. Dalton. Trans. 39, 3657–3659]. The intermolecular hydrogen bond distances and bond angles were listed in table 2.

Experimental

2-Hydroxyaniline(1 mmol, 109.12 mg) and potassium hydroxide (1 mmol, 56.1 mg) were dissolved in hot methanol (10 ml) and added dropwise to a methanol solution of *o*-vanillin (1 mmol, 152.2 mg). The mixture was then stirred at 323 K for 2 h. Subsequently, an aqueous solution(2 ml) of cupric acetate monohydrate(1 mmol, 199.7 mg) was added dropwise and stirred for 2 h. An methanol solution (5 ml) of phenanthroline(1 mmol, 198.2 mg) was added dropwise and stirred for 4 h. The solution was held at room temperature for ten days, whereupon green blocky crystals suitable for X-ray diffraction analysis were obtained.

Refinement

Difference Fourier maps revealed that the methanol molecule is disordered between two positions. The subsequent refinement of their occupancies gave the values of 0.566 (4) and 0.434 (4), respectively. All H atoms were placed in geometrically

calculated positions (O—H = 0.82 Å, C—H = 0.93 − 0.97 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2–1.5U_{eq}(parent atom).

Figures

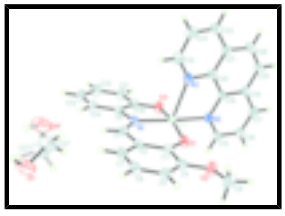

Fig. 1. The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

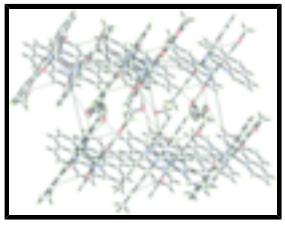

Fig. 2. Packing diagram of the title compound.

[2-(3-Methoxy-2-oxidobenzylideneamino)phenolato-κ^3*O*,*N*,*O*'](1,10- phenanthroline-κ^2*N*,*N*')copper(II) methanol solvate

Crystal data

$[Cu(C_{14}H_{11}NO_3)(C_{12}H_8N_2)]\cdot C_1H_4O$	$Z = 2$
$M_r = 517.02$	$F_{000} = 534$
Triclinic, $P\overline{1}$	$D_x = 1.482$ Mg m^{-3}
$a = 9.905$ (3) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.335$ (3) Å	Cell parameters from 2789 reflections
$c = 12.094$ (3) Å	$\theta = 2.3$–27.6º
$\alpha = 82.701$ (3)º	$\mu = 0.98$ mm^{-1}
$\beta = 70.742$ (3)º	$T = 298$ (2) K
$\gamma = 89.236$ (3)º	Block, blue
$V = 1158.8$ (6) Å^3	0.21 × 0.18 × 0.07 mm

Data collection

Siemens SMART CCD area-detector diffractometer	4012 independent reflections
Radiation source: fine-focus sealed tube	3134 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.018$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SABADS; Sheldrick, 1996)	$h = -11 \rightarrow 8$
$T_{min} = 0.820$, $T_{max} = 0.934$	$k = -11 \rightarrow 12$

5996 measured reflections

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.096$

$S = 1.03$

4012 reflections

325 parameters

16 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.4525P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.48$ e Å^{-3}

$\Delta\rho_{min} = -0.46$ e Å^{-3}

Extinction correction: none

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	−0.06105 (4)	0.81675 (4)	0.73686 (3)	0.03642 (14)	
N1	−0.0446 (2)	0.7433 (2)	0.5923 (2)	0.0349 (6)	
N2	−0.1087 (3)	0.8788 (2)	0.8987 (2)	0.0346 (6)	
N3	0.0767 (3)	0.6863 (2)	0.8276 (2)	0.0416 (6)	
O1	0.0849 (2)	0.9503 (2)	0.65842 (16)	0.0433 (5)	
O2	0.2853 (3)	1.1329 (2)	0.5911 (2)	0.0594 (7)	
O3	−0.2347 (2)	0.7071 (2)	0.80315 (17)	0.0447 (5)	
O4	0.5173 (6)	0.8061 (5)	−0.0646 (4)	0.0833 (13)	0.566 (4)
H4	0.5785	0.7648	−0.1087	0.125*	0.566 (4)
O4'	0.5881 (8)	0.6913 (7)	0.0324 (5)	0.0833 (13)	0.434 (4)
H4'	0.6469	0.6899	−0.0335	0.125*	0.434 (4)
C1	0.0500 (3)	0.7797 (3)	0.4913 (3)	0.0395 (7)	
H1	0.0473	0.7368	0.4289	0.047*	
C2	0.1585 (3)	0.8789 (3)	0.4651 (2)	0.0353 (7)	
C3	0.1689 (3)	0.9587 (3)	0.5493 (2)	0.0359 (7)	
C4	0.2815 (3)	1.0569 (3)	0.5073 (3)	0.0406 (7)	

C5	0.3739 (3)	1.0715 (3)	0.3943 (3)	0.0482 (8)	
H5	0.4456	1.1363	0.3703	0.058*	
C6	0.3617 (4)	0.9898 (3)	0.3138 (3)	0.0531 (9)	
H6	0.4253	0.9998	0.2369	0.064*	
C7	0.2572 (3)	0.8969 (3)	0.3489 (3)	0.0473 (8)	
H7	0.2496	0.8429	0.2952	0.057*	
C8	0.4035 (4)	1.2217 (4)	0.5636 (3)	0.0674 (11)	
H8A	0.4909	1.1752	0.5408	0.101*	
H8B	0.3971	1.2633	0.6317	0.101*	
H8C	0.4024	1.2866	0.4997	0.101*	
C9	−0.1522 (3)	0.6459 (3)	0.6113 (3)	0.0358 (7)	
C10	−0.2511 (3)	0.6329 (3)	0.7263 (3)	0.0391 (7)	
C11	−0.3634 (4)	0.5416 (3)	0.7559 (3)	0.0535 (9)	
H11	−0.4313	0.5328	0.8311	0.064*	
C12	−0.3746 (4)	0.4638 (3)	0.6740 (3)	0.0601 (10)	
H12	−0.4495	0.4024	0.6950	0.072*	
C13	−0.2762 (4)	0.4765 (3)	0.5618 (3)	0.0561 (9)	
H13	−0.2846	0.4236	0.5075	0.067*	
C14	−0.1655 (4)	0.5674 (3)	0.5301 (3)	0.0467 (8)	
H14	−0.0993	0.5763	0.4541	0.056*	
C15	−0.2009 (3)	0.9712 (3)	0.9343 (3)	0.0411 (8)	
H15	−0.2401	1.0152	0.8807	0.049*	
C16	−0.2419 (3)	1.0055 (3)	1.0479 (3)	0.0454 (8)	
H16	−0.3066	1.0715	1.0690	0.054*	
C17	−0.1867 (3)	0.9419 (3)	1.1279 (3)	0.0456 (8)	
H17	−0.2122	0.9646	1.2039	0.055*	
C18	−0.0906 (3)	0.8415 (3)	1.0944 (3)	0.0402 (7)	
C19	−0.0542 (3)	0.8127 (3)	0.9781 (2)	0.0335 (7)	
C20	0.0459 (3)	0.7120 (3)	0.9396 (3)	0.0371 (7)	
C21	0.1055 (3)	0.6438 (3)	1.0203 (3)	0.0438 (8)	
C22	0.2003 (4)	0.5448 (4)	0.9792 (3)	0.0552 (9)	
H22	0.2415	0.4962	1.0293	0.066*	
C23	0.2313 (4)	0.5208 (4)	0.8663 (3)	0.0601 (10)	
H23	0.2950	0.4563	0.8380	0.072*	
C24	0.1679 (4)	0.5926 (3)	0.7929 (3)	0.0519 (9)	
H24	0.1904	0.5741	0.7156	0.062*	
C25	−0.0268 (4)	0.7709 (3)	1.1735 (3)	0.0492 (9)	
H25	−0.0500	0.7906	1.2504	0.059*	
C26	0.0663 (4)	0.6767 (4)	1.1375 (3)	0.0537 (9)	
H26	0.1060	0.6318	1.1904	0.064*	
C27	0.4951 (14)	0.7539 (17)	0.0535 (10)	0.071 (3)	0.566 (4)
H27A	0.5828	0.7600	0.0702	0.106*	0.566 (4)
H27B	0.4640	0.6641	0.0657	0.106*	0.566 (4)
H27C	0.4231	0.8021	0.1051	0.106*	0.566 (4)
C27'	0.4749 (19)	0.763 (2)	0.0235 (16)	0.071 (3)	0.434 (4)
H27D	0.3924	0.7384	0.0917	0.106*	0.434 (4)
H27E	0.4550	0.7481	−0.0464	0.106*	0.434 (4)
H27F	0.4976	0.8543	0.0189	0.106*	0.434 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0389 (2)	0.0426 (2)	0.0274 (2)	−0.00479 (16)	−0.00977 (15)	−0.00596 (15)
N1	0.0341 (14)	0.0396 (15)	0.0318 (13)	−0.0005 (11)	−0.0120 (11)	−0.0050 (11)
N2	0.0365 (14)	0.0348 (14)	0.0334 (13)	−0.0032 (12)	−0.0124 (11)	−0.0045 (11)
N3	0.0432 (15)	0.0452 (16)	0.0351 (14)	0.0008 (13)	−0.0100 (12)	−0.0088 (12)
O1	0.0475 (13)	0.0502 (13)	0.0290 (11)	−0.0100 (11)	−0.0069 (10)	−0.0080 (9)
O2	0.0668 (16)	0.0581 (15)	0.0511 (14)	−0.0235 (13)	−0.0146 (12)	−0.0098 (12)
O3	0.0424 (12)	0.0521 (14)	0.0361 (12)	−0.0118 (10)	−0.0054 (10)	−0.0125 (10)
O4	0.071 (3)	0.095 (3)	0.061 (3)	0.031 (2)	0.000 (2)	0.012 (2)
O4'	0.071 (3)	0.095 (3)	0.061 (3)	0.031 (2)	0.000 (2)	0.012 (2)
C1	0.0439 (18)	0.0439 (19)	0.0333 (17)	0.0040 (15)	−0.0154 (15)	−0.0077 (14)
C2	0.0377 (16)	0.0393 (18)	0.0281 (15)	0.0018 (14)	−0.0113 (13)	−0.0001 (13)
C3	0.0363 (17)	0.0404 (18)	0.0316 (16)	0.0018 (14)	−0.0141 (14)	0.0004 (13)
C4	0.0427 (18)	0.0424 (19)	0.0383 (17)	0.0005 (15)	−0.0165 (15)	−0.0025 (14)
C5	0.0424 (19)	0.050 (2)	0.0457 (19)	−0.0093 (16)	−0.0114 (16)	0.0078 (16)
C6	0.051 (2)	0.067 (2)	0.0314 (17)	−0.0069 (18)	−0.0030 (15)	0.0005 (16)
C7	0.049 (2)	0.059 (2)	0.0321 (17)	−0.0061 (17)	−0.0113 (15)	−0.0047 (15)
C8	0.065 (3)	0.060 (3)	0.080 (3)	−0.019 (2)	−0.027 (2)	−0.009 (2)
C9	0.0352 (16)	0.0359 (17)	0.0388 (16)	0.0027 (13)	−0.0156 (13)	−0.0054 (13)
C10	0.0364 (17)	0.0404 (18)	0.0414 (17)	−0.0006 (14)	−0.0144 (14)	−0.0049 (14)
C11	0.046 (2)	0.056 (2)	0.053 (2)	−0.0122 (17)	−0.0077 (16)	−0.0098 (17)
C12	0.056 (2)	0.053 (2)	0.071 (3)	−0.0169 (18)	−0.020 (2)	−0.0122 (19)
C13	0.062 (2)	0.053 (2)	0.060 (2)	−0.0067 (18)	−0.0230 (19)	−0.0223 (18)
C14	0.049 (2)	0.048 (2)	0.0442 (18)	−0.0016 (16)	−0.0146 (16)	−0.0132 (15)
C15	0.0434 (19)	0.0426 (19)	0.0400 (17)	−0.0030 (16)	−0.0182 (15)	−0.0026 (14)
C16	0.048 (2)	0.0427 (19)	0.0454 (19)	0.0051 (16)	−0.0133 (16)	−0.0131 (15)
C17	0.053 (2)	0.050 (2)	0.0331 (17)	−0.0025 (17)	−0.0111 (15)	−0.0115 (15)
C18	0.0444 (18)	0.0441 (19)	0.0340 (16)	−0.0045 (15)	−0.0153 (14)	−0.0055 (14)
C19	0.0333 (16)	0.0381 (17)	0.0303 (15)	−0.0062 (13)	−0.0129 (13)	−0.0015 (13)
C20	0.0345 (17)	0.0398 (18)	0.0368 (17)	−0.0032 (14)	−0.0123 (14)	−0.0028 (14)
C21	0.0383 (18)	0.049 (2)	0.0465 (19)	−0.0011 (16)	−0.0181 (15)	−0.0021 (15)
C22	0.047 (2)	0.061 (2)	0.063 (2)	0.0084 (18)	−0.0269 (18)	−0.0029 (19)
C23	0.048 (2)	0.061 (2)	0.070 (3)	0.0153 (19)	−0.0162 (19)	−0.017 (2)
C24	0.051 (2)	0.060 (2)	0.0423 (19)	0.0034 (19)	−0.0092 (17)	−0.0137 (17)
C25	0.058 (2)	0.060 (2)	0.0344 (17)	0.0011 (19)	−0.0217 (16)	−0.0050 (16)
C26	0.060 (2)	0.066 (2)	0.0429 (19)	0.002 (2)	−0.0297 (18)	0.0011 (17)
C27	0.051 (4)	0.087 (4)	0.065 (6)	0.004 (4)	−0.017 (4)	0.011 (5)
C27'	0.051 (4)	0.087 (4)	0.065 (6)	0.004 (4)	−0.017 (4)	0.011 (5)

Geometric parameters (Å, °)

Cu1—O1	1.926 (2)	C10—C11	1.391 (4)
Cu1—O3	1.949 (2)	C11—C12	1.385 (4)
Cu1—N1	1.950 (2)	C11—H11	0.9300
Cu1—N2	2.041 (2)	C12—C13	1.376 (5)
Cu1—N3	2.333 (3)	C12—H12	0.9300

N1—C1	1.284 (4)	C13—C14	1.375 (4)
N1—C9	1.419 (3)	C13—H13	0.9300
N2—C15	1.324 (4)	C14—H14	0.9300
N2—C19	1.359 (4)	C15—C16	1.389 (4)
N3—C24	1.327 (4)	C15—H15	0.9300
N3—C20	1.347 (4)	C16—C17	1.359 (4)
O1—C3	1.300 (3)	C16—H16	0.9300
O2—C4	1.369 (3)	C17—C18	1.404 (4)
O2—C8	1.421 (4)	C17—H17	0.9300
O3—C10	1.328 (3)	C18—C19	1.402 (4)
O4—C27	1.407 (11)	C18—C25	1.434 (4)
O4—H4	0.8200	C19—C20	1.440 (4)
O4'—C27'	1.364 (15)	C20—C21	1.412 (4)
O4'—H4'	0.8200	C21—C22	1.404 (5)
C1—C2	1.425 (4)	C21—C26	1.425 (4)
C1—H1	0.9300	C22—C23	1.352 (5)
C2—C7	1.413 (4)	C22—H22	0.9300
C2—C3	1.418 (4)	C23—C24	1.386 (5)
C3—C4	1.434 (4)	C23—H23	0.9300
C4—C5	1.361 (4)	C24—H24	0.9300
C5—C6	1.401 (4)	C25—C26	1.345 (5)
C5—H5	0.9300	C25—H25	0.9300
C6—C7	1.344 (4)	C26—H26	0.9300
C6—H6	0.9300	C27—H27A	0.9600
C7—H7	0.9300	C27—H27B	0.9600
C8—H8A	0.9600	C27—H27C	0.9600
C8—H8B	0.9600	C27'—H27D	0.9600
C8—H8C	0.9600	C27'—H27E	0.9600
C9—C14	1.390 (4)	C27'—H27F	0.9600
C9—C10	1.403 (4)		
O1—Cu1—O3	167.67 (9)	C10—C11—H11	119.8
O1—Cu1—N1	94.04 (9)	C13—C12—C11	120.7 (3)
O3—Cu1—N1	83.92 (9)	C13—C12—H12	119.6
O1—Cu1—N2	94.42 (8)	C11—C12—H12	119.6
O3—Cu1—N2	87.19 (9)	C14—C13—C12	119.9 (3)
N1—Cu1—N2	171.06 (9)	C14—C13—H13	120.0
O1—Cu1—N3	96.12 (9)	C12—C13—H13	120.0
O3—Cu1—N3	96.14 (9)	C13—C14—C9	120.1 (3)
N1—Cu1—N3	105.59 (9)	C13—C14—H14	119.9
N2—Cu1—N3	76.37 (9)	C9—C14—H14	119.9
C1—N1—C9	123.6 (2)	N2—C15—C16	123.2 (3)
C1—N1—Cu1	124.6 (2)	N2—C15—H15	118.4
C9—N1—Cu1	111.79 (18)	C16—C15—H15	118.4
C15—N2—C19	118.2 (3)	C17—C16—C15	119.4 (3)
C15—N2—Cu1	123.4 (2)	C17—C16—H16	120.3
C19—N2—Cu1	118.0 (2)	C15—C16—H16	120.3
C24—N3—C20	117.6 (3)	C16—C17—C18	119.3 (3)
C24—N3—Cu1	133.2 (2)	C16—C17—H17	120.4
C20—N3—Cu1	109.1 (2)	C18—C17—H17	120.4

C3—O1—Cu1	125.68 (18)	C19—C18—C17	118.0 (3)
C4—O2—C8	117.9 (3)	C19—C18—C25	119.5 (3)
C10—O3—Cu1	111.84 (18)	C17—C18—C25	122.5 (3)
C27'—O4'—H4'	109.5	N2—C19—C18	121.9 (3)
N1—C1—C2	126.6 (3)	N2—C19—C20	118.3 (2)
N1—C1—H1	116.7	C18—C19—C20	119.8 (3)
C2—C1—H1	116.7	N3—C20—C21	123.0 (3)
C7—C2—C3	120.2 (3)	N3—C20—C19	117.9 (3)
C7—C2—C1	116.9 (3)	C21—C20—C19	119.1 (3)
C3—C2—C1	122.9 (3)	C22—C21—C20	116.9 (3)
O1—C3—C2	125.4 (3)	C22—C21—C26	123.7 (3)
O1—C3—C4	118.8 (3)	C20—C21—C26	119.4 (3)
C2—C3—C4	115.8 (3)	C23—C22—C21	119.4 (3)
C5—C4—O2	124.3 (3)	C23—C22—H22	120.3
C5—C4—C3	122.2 (3)	C21—C22—H22	120.3
O2—C4—C3	113.5 (3)	C22—C23—C24	119.9 (3)
C4—C5—C6	120.6 (3)	C22—C23—H23	120.1
C4—C5—H5	119.7	C24—C23—H23	120.1
C6—C5—H5	119.7	N3—C24—C23	123.1 (3)
C7—C6—C5	119.4 (3)	N3—C24—H24	118.5
C7—C6—H6	120.3	C23—C24—H24	118.5
C5—C6—H6	120.3	C26—C25—C18	120.6 (3)
C6—C7—C2	121.9 (3)	C26—C25—H25	119.7
C6—C7—H7	119.0	C18—C25—H25	119.7
C2—C7—H7	119.0	C25—C26—C21	121.6 (3)
O2—C8—H8A	109.5	C25—C26—H26	119.2
O2—C8—H8B	109.5	C21—C26—H26	119.2
H8A—C8—H8B	109.5	O4—C27—H27A	109.5
O2—C8—H8C	109.5	O4—C27—H27B	109.5
H8A—C8—H8C	109.5	H27A—C27—H27B	109.5
H8B—C8—H8C	109.5	O4—C27—H27C	109.5
C14—C9—C10	120.4 (3)	H27A—C27—H27C	109.5
C14—C9—N1	126.9 (3)	H27B—C27—H27C	109.5
C10—C9—N1	112.7 (2)	O4'—C27'—H27D	109.5
O3—C10—C11	122.2 (3)	O4'—C27'—H27E	109.5
O3—C10—C9	119.4 (3)	H27D—C27'—H27E	109.5
C11—C10—C9	118.4 (3)	O4'—C27'—H27F	109.5
C12—C11—C10	120.4 (3)	H27D—C27'—H27F	109.5
C12—C11—H11	119.8	H27E—C27'—H27F	109.5
O1—Cu1—N1—C1	5.8 (3)	C1—N1—C9—C14	6.3 (5)
O3—Cu1—N1—C1	173.6 (3)	Cu1—N1—C9—C14	−174.9 (3)
N2—Cu1—N1—C1	166.8 (6)	C1—N1—C9—C10	−174.0 (3)
N3—Cu1—N1—C1	−91.7 (3)	Cu1—N1—C9—C10	4.8 (3)
O1—Cu1—N1—C9	−172.97 (19)	Cu1—O3—C10—C11	176.6 (3)
O3—Cu1—N1—C9	−5.18 (19)	Cu1—O3—C10—C9	−3.3 (3)
N2—Cu1—N1—C9	−12.0 (7)	C14—C9—C10—O3	178.7 (3)
N3—Cu1—N1—C9	89.52 (19)	N1—C9—C10—O3	−1.0 (4)
O1—Cu1—N2—C15	86.0 (2)	C14—C9—C10—C11	−1.2 (5)
O3—Cu1—N2—C15	−81.8 (2)	N1—C9—C10—C11	179.1 (3)

N1—Cu1—N2—C15	−75.0 (7)	O3—C10—C11—C12	−178.4 (3)
N3—Cu1—N2—C15	−178.8 (2)	C9—C10—C11—C12	1.4 (5)
O1—Cu1—N2—C19	−101.1 (2)	C10—C11—C12—C13	−0.8 (6)
O3—Cu1—N2—C19	91.2 (2)	C11—C12—C13—C14	−0.1 (6)
N1—Cu1—N2—C19	97.9 (7)	C12—C13—C14—C9	0.4 (5)
N3—Cu1—N2—C19	−5.86 (19)	C10—C9—C14—C13	0.2 (5)
O1—Cu1—N3—C24	−86.5 (3)	N1—C9—C14—C13	179.9 (3)
O3—Cu1—N3—C24	94.8 (3)	C19—N2—C15—C16	1.5 (4)
N1—Cu1—N3—C24	9.4 (3)	Cu1—N2—C15—C16	174.5 (2)
N2—Cu1—N3—C24	−179.6 (3)	N2—C15—C16—C17	−0.4 (5)
O1—Cu1—N3—C20	97.58 (19)	C15—C16—C17—C18	−0.8 (5)
O3—Cu1—N3—C20	−81.09 (19)	C16—C17—C18—C19	0.9 (4)
N1—Cu1—N3—C20	−166.48 (19)	C16—C17—C18—C25	179.3 (3)
N2—Cu1—N3—C20	4.50 (18)	C15—N2—C19—C18	−1.4 (4)
O3—Cu1—O1—C3	−88.9 (5)	Cu1—N2—C19—C18	−174.7 (2)
N1—Cu1—O1—C3	−8.9 (2)	C15—N2—C19—C20	179.9 (3)
N2—Cu1—O1—C3	174.0 (2)	Cu1—N2—C19—C20	6.6 (3)
N3—Cu1—O1—C3	97.3 (2)	C17—C18—C19—N2	0.2 (4)
O1—Cu1—O3—C10	85.7 (4)	C25—C18—C19—N2	−178.3 (3)
N1—Cu1—O3—C10	4.7 (2)	C17—C18—C19—C20	178.9 (3)
N2—Cu1—O3—C10	−176.4 (2)	C25—C18—C19—C20	0.4 (4)
N3—Cu1—O3—C10	−100.4 (2)	C24—N3—C20—C21	−0.3 (4)
C9—N1—C1—C2	178.3 (3)	Cu1—N3—C20—C21	176.3 (2)
Cu1—N1—C1—C2	−0.4 (4)	C24—N3—C20—C19	−179.3 (3)
N1—C1—C2—C7	176.1 (3)	Cu1—N3—C20—C19	−2.7 (3)
N1—C1—C2—C3	−4.8 (5)	N2—C19—C20—N3	−2.0 (4)
Cu1—O1—C3—C2	6.7 (4)	C18—C19—C20—N3	179.2 (3)
Cu1—O1—C3—C4	−174.0 (2)	N2—C19—C20—C21	178.9 (2)
C7—C2—C3—O1	−179.5 (3)	C18—C19—C20—C21	0.2 (4)
C1—C2—C3—O1	1.4 (5)	N3—C20—C21—C22	−0.3 (4)
C7—C2—C3—C4	1.2 (4)	C19—C20—C21—C22	178.7 (3)
C1—C2—C3—C4	−177.9 (3)	N3—C20—C21—C26	−179.5 (3)
C8—O2—C4—C5	−8.3 (5)	C19—C20—C21—C26	−0.5 (4)
C8—O2—C4—C3	172.0 (3)	C20—C21—C22—C23	0.9 (5)
O1—C3—C4—C5	179.9 (3)	C26—C21—C22—C23	−179.9 (3)
C2—C3—C4—C5	−0.8 (4)	C21—C22—C23—C24	−0.9 (5)
O1—C3—C4—O2	−0.5 (4)	C20—N3—C24—C23	0.3 (5)
C2—C3—C4—O2	178.9 (3)	Cu1—N3—C24—C23	−175.3 (2)
O2—C4—C5—C6	−179.6 (3)	C22—C23—C24—N3	0.3 (5)
C3—C4—C5—C6	0.0 (5)	C19—C18—C25—C26	−0.7 (5)
C4—C5—C6—C7	0.4 (5)	C17—C18—C25—C26	−179.1 (3)
C5—C6—C7—C2	0.0 (5)	C18—C25—C26—C21	0.3 (5)
C3—C2—C7—C6	−0.8 (5)	C22—C21—C26—C25	−178.9 (3)
C1—C2—C7—C6	178.3 (3)	C20—C21—C26—C25	0.3 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O3^{i}	0.82	1.93	2.719 (5)	160

O4'—H4'···O3^{i}	0.82	1.92	2.735 (6)	171
C17—H17···O2^{ii}	0.93	2.43	3.204 (4)	141

Symmetry codes: (i) *x*+1, *y*, *z*−1; (ii) −*x*, −*y*+2, −*z*+2.

Fig. 1

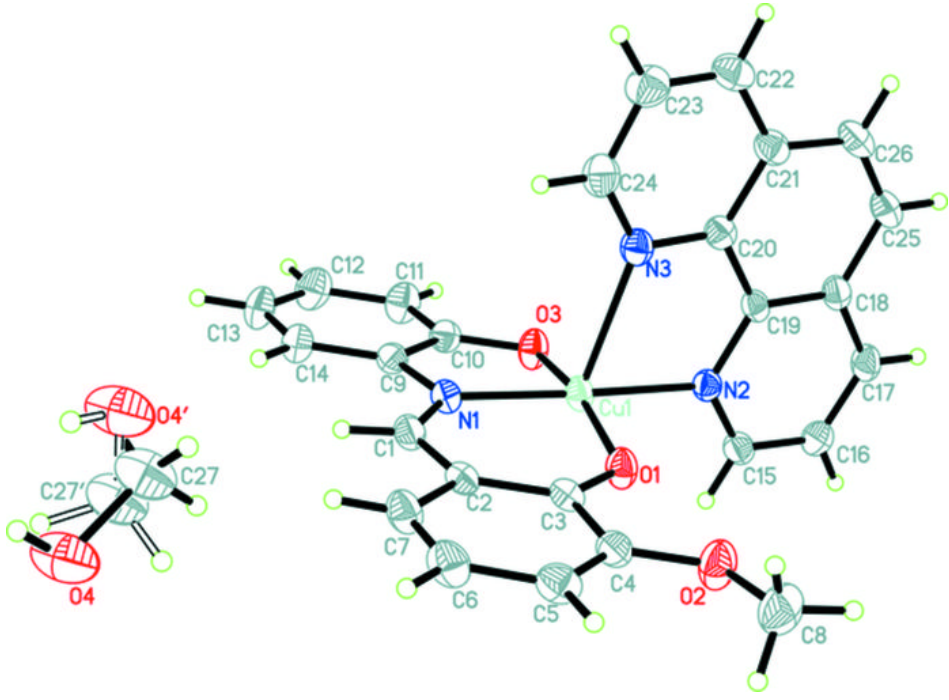
C22
C23
C26
C21
C24
C25
N3
C20
C12
C11
C18
C19
O3
C13
C10
C14
C9
N2
C17
N1
Cu1
C1
O1
C16
C15
C2
C3
C7
C4
O2
C6
C5
C8
O4'
C27
C27'
O4

Fig. 2