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(2,2′-Bipyridine-κ^2N,N')[3-(2-oxidobenzylideneamino)propanoato-κ^3O,N,O']copper(II) dihydrate

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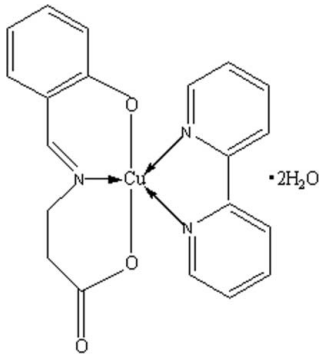
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.029; wR factor = 0.080; data-to-parameter ratio = 12.3.

In the title compound, $[Cu(C_{10}H_9NO_3)(C_{10}H_8N_2)]\cdot 2H_2O$, the Cu^{II} atom is five-coordinated in a distorted square-pyramidal geometry. The basal positions are occupied by three donor atoms from the tridentate Schiff base ligand and by one N atom from a 2,2′-bipyridine ligand. The apical position is occupied by the other N atom of the 2,2′-bipyridine ligand. The solvent water molecules link adjacent complex molecules through O—H···O hydrogen bonds into a chain running along the [$\bar{1}$01] direction.

Related literature

For synthesis, see: Plesch *et al.* (1997). For related literature, see: Raso *et al.* (1996, 1999). For related structures, see: Reddy *et al.* (2002); Wang *et al.* (2005); Warda (1997, 1998*a*,*b*,*c*).



Experimental

Crystal data

$[Cu(C_{10}H_9NO_3)(C_{10}H_8N_2)]\cdot 2H_2O$
M_r = 446.94
Monoclinic, $C2/c$
a = 15.1164 (14) Å
b = 13.1426 (12) Å
c = 19.6898 (19) Å
β = 91.204 (1)°
V = 3910.9 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.16 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.723, T_{max} = 0.802
9940 measured reflections
3427 independent reflections
2954 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.080
S = 1.04
3427 reflections
279 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9475 (16)	Cu1—N1	2.0261 (17)
Cu1—N3	1.9492 (17)	Cu1—N2	2.2429 (17)
Cu1—O2	1.9715 (17)		
O1—Cu1—N3	92.45 (7)	O2—Cu1—N1	86.08 (7)
O1—Cu1—O2	158.33 (8)	O1—Cu1—N2	94.25 (7)
N3—Cu1—O2	92.82 (7)	N3—Cu1—N2	105.81 (7)
O1—Cu1—N1	87.53 (7)	O2—Cu1—N2	104.48 (7)
N3—Cu1—N1	176.87 (7)	N1—Cu1—N2	77.31 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O2^{i}	0.842 (10)	2.34 (3)	3.075 (4)	146 (5)
O4—H4B···O1	0.847 (10)	1.96 (1)	2.801 (3)	174 (3)
O5—H5B···O3	0.842 (10)	1.99 (2)	2.794 (4)	160 (5)

Symmetry code: (i) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 2000); 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: CI2408).

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supplementary materials

Acta Cryst. (2007). E**63**, m2351-m2352 [**doi:10.1107/S1600536807034691**]

(2,2'-Bipyridine-κ^2N,N')[3-(2-oxidobenzylideneamino)propanoato-κ^3O,N,O']copper(II) dihydrate

J.-M. Xie, G.-Q. Zhao, M. Shao, H. Liu and X.-J. Lu

Comment

Considerable efforts have been devoted to copper(II) complexes of tridentate Schiff base ligands of *N*-alkylidene or *N*-arylidene aminoacidato type due to their structural richness, electrochemical properties as well as a potential model for a number of important biological systems (Raso *et al.*, 1996, 1999). Several stuctural studies have been performed on Schiff base copper(II) complexes derived from salicylaldehyde and animo acids (Reddy *et al.*, 2002; Wang *et al.*, 2005; Warda, 1997, 1998*a*,b,c). We report here the crystal structure of the title Cu^{II} complex.

The structure consists of discrete monomeric square-pyramidal Cu^{II} complex (Fig. 1 and Table 1). The basal positions are occupied by three donor atoms from the tridentate Schiff base ligand, which furnishes an ONO donor set, with the fourth position occupied by one N atom from the 2,2'-bipyridine ligand. The axial position is occupied by the other N atom of the 2,2'-bipyridine igand. The Cu atom is displaced from the O1/O2/N1/N3 basal plane toward the N2 atom by 0.2038 (2) Å.

The 2,2'-bipyridine ligand is essentially planar and it forms a dihedral angle of 81.95 (10)° with the benzene ring of the Schiff base ligand.

The crystal structure is stabilized by O—H···O type hydrogen bonds (Table 2). The lattice water molecules link adjacent complex molecules through O—H···O hydrogen bonds into a chain running along the [$\bar{1}$ 0 1] direction (Fig. 2). The closest Cu···Cu separation in the chain is 5.701 Å.

Experimental

The title compound was synthesized by a literature method (Plesch *et al.*, 1997). The method of synthesis was as follows: To a solution of β-alanine (1 mmol) and lithium hydroxide monohydrate (1 mmol) in methanol (10 ml) was added a solution of salicylaldehyde (1 mmol) in methanol(10 ml). The yellow solution was stirred for 1 h at room temperature prior to cooling in an ice bath. The resultant mixture was added dropwise to a mixture of copper(II) acetate monohydrate (1 mmol) and 2,2'-bipyridine (1 mmol) in an aqueous methanolic solution (20 ml, 1:1 *v*/*v*), and heated with stirring for 2 h at 333 K. The dark green solution was filtered and left for several days. The resulting dark-blue crystals were filtered off, washed with water, and dried under vacuum. Analysis found: C 53.75, H 4.74, N 9.40%; calculated: C 53.29, H 4.56, N 9.77%.

Refinement

The water H atoms were located in a difference Fourier map and were refined with distance restraints of O—H = 0.84 (1) Å and H···H = 1.37 (2) Å. C-bound H atoms were placed in geometrically idealized positions (C—H = 0.93 or 0.97 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

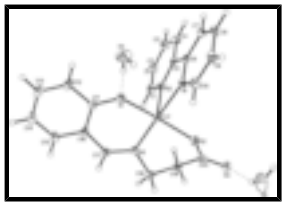

Fig. 1. Molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bonds are shown as dashed lines.

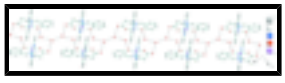

Fig. 2. Part of a hydrogen-bonded (dashed lines) chain of the title compound.

(2,2'-Bipyridine-κ^2N,N')[3-(2-oxidobenzylideneamino)propanoato- κ^3O,N,O']copper(II) dihydrate

Crystal data

$[Cu(C_{10}H_9NO_3)(C_{10}H_8N_2)]\cdot 2H_2O$	F_{000} = 1848
M_r = 446.94	D_x = 1.518 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4685 reflections
a = 15.1164 (14) Å	θ = 2.3–26.8º
b = 13.1426 (12) Å	μ = 1.16 mm^{-1}
c = 19.6898 (19) Å	*T* = 298 (2) K
β = 91.204 (1)º	Block, dark green
V = 3910.9 (6) Å^3	0.30 × 0.20 × 0.20 mm
Z = 8	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	3427 independent reflections
Radiation source: fine-focus sealed tube	2954 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −17→12
T_{min} = 0.723, T_{max} = 0.802	*k* = −14→15
9940 measured reflections	*l* = −23→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H atoms treated by a mixture of independent and constrained refinement

$wR(F^2) = 0.080$	$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 2.2382P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.002$
3427 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
279 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}
6 restraints	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00067 (11)

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}
Cu1	0.087909 (17)	0.740584 (18)	0.423632 (12)	0.03594 (12)
C1	−0.05975 (15)	0.62930 (18)	0.32611 (11)	0.0488 (6)
H1	−0.0767	0.6942	0.3123	0.059*
C2	−0.10048 (18)	0.5472 (2)	0.29577 (13)	0.0599 (7)
H2	−0.1442	0.5560	0.2623	0.072*
C3	−0.07487 (19)	0.4520 (2)	0.31624 (14)	0.0643 (7)
H3	−0.1010	0.3949	0.2965	0.077*
C4	−0.01062 (18)	0.44065 (18)	0.36590 (13)	0.0551 (6)
H4	0.0066	0.3762	0.3805	0.066*
C5	0.02824 (14)	0.52682 (15)	0.39396 (10)	0.0379 (5)
C6	0.09825 (14)	0.52231 (15)	0.44798 (10)	0.0369 (5)
C7	0.13000 (17)	0.43154 (17)	0.47509 (12)	0.0517 (6)
H7	0.1083	0.3697	0.4588	0.062*
C8	0.19355 (17)	0.4334 (2)	0.52598 (13)	0.0580 (7)
H8	0.2157	0.3729	0.5440	0.070*
C9	0.22382 (17)	0.5243 (2)	0.54970 (13)	0.0598 (7)
H9	0.2662	0.5272	0.5845	0.072*
C10	0.19027 (16)	0.61197 (19)	0.52099 (12)	0.0536 (6)
H10	0.2106	0.6742	0.5374	0.064*
C11	0.19829 (15)	0.77373 (17)	0.30493 (11)	0.0424 (5)
C12	0.26208 (17)	0.7385 (2)	0.25875 (14)	0.0548 (6)
H12	0.2924	0.6784	0.2681	0.066*
C13	0.28013 (18)	0.7913 (3)	0.20050 (13)	0.0655 (7)

H13	0.3219	0.7657	0.1710	0.079*
C14	0.23770 (18)	0.8812 (2)	0.18480 (13)	0.0660 (8)
H14	0.2518	0.9173	0.1459	0.079*
C15	0.17490 (17)	0.9164 (2)	0.22715 (12)	0.0559 (6)
H15	0.1458	0.9769	0.2165	0.067*
C16	0.15252 (14)	0.86370 (17)	0.28690 (10)	0.0418 (5)
C17	0.08414 (15)	0.90614 (16)	0.32727 (11)	0.0440 (5)
H17	0.0604	0.9677	0.3124	0.053*
C18	−0.01486 (18)	0.93121 (18)	0.41580 (12)	0.0564 (7)
H18A	−0.0445	0.9742	0.3823	0.068*
H18B	0.0147	0.9752	0.4486	0.068*
C19	−0.08308 (16)	0.86842 (19)	0.45159 (12)	0.0537 (6)
H19A	−0.1317	0.9122	0.4642	0.064*
H19B	−0.1064	0.8174	0.4204	0.064*
C20	−0.04692 (16)	0.81623 (16)	0.51415 (11)	0.0458 (5)
N1	0.12982 (12)	0.61166 (13)	0.47065 (9)	0.0392 (4)
N2	0.00289 (12)	0.62053 (13)	0.37434 (8)	0.0386 (4)
N3	0.05187 (12)	0.86882 (12)	0.38171 (9)	0.0397 (4)
O1	0.18482 (11)	0.72290 (12)	0.36108 (9)	0.0495 (4)
O2	0.02817 (13)	0.77239 (13)	0.50911 (8)	0.0566 (5)
O3	−0.08925 (12)	0.81717 (15)	0.56686 (8)	0.0650 (5)
O4	0.33568 (19)	0.6129 (2)	0.40144 (16)	0.1006 (8)
O5	0.0196 (2)	0.8368 (3)	0.68258 (17)	0.1303 (11)
H4A	0.357 (3)	0.636 (4)	0.4383 (17)	0.21 (3)*
H4B	0.2906 (15)	0.649 (2)	0.3917 (17)	0.109 (13)*
H5B	−0.020 (2)	0.842 (3)	0.6523 (19)	0.18 (2)*
H5A	0.019 (2)	0.7785 (12)	0.6976 (15)	0.175 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03707 (18)	0.03392 (16)	0.03682 (17)	0.00184 (10)	0.00015 (11)	0.00119 (10)
C1	0.0478 (14)	0.0539 (14)	0.0445 (13)	0.0022 (11)	−0.0044 (11)	0.0002 (10)
C2	0.0521 (16)	0.0751 (18)	0.0519 (15)	−0.0081 (14)	−0.0098 (12)	−0.0098 (13)
C3	0.0676 (18)	0.0602 (16)	0.0647 (17)	−0.0211 (14)	−0.0041 (14)	−0.0147 (13)
C4	0.0631 (16)	0.0423 (13)	0.0599 (15)	−0.0082 (12)	0.0027 (13)	−0.0037 (11)
C5	0.0383 (12)	0.0373 (11)	0.0384 (11)	−0.0011 (9)	0.0103 (9)	−0.0020 (9)
C6	0.0356 (11)	0.0391 (11)	0.0365 (11)	0.0040 (9)	0.0104 (9)	0.0039 (9)
C7	0.0589 (15)	0.0406 (12)	0.0560 (15)	0.0061 (11)	0.0133 (12)	0.0069 (10)
C8	0.0527 (15)	0.0612 (16)	0.0605 (16)	0.0184 (13)	0.0066 (13)	0.0249 (13)
C9	0.0491 (15)	0.0760 (18)	0.0539 (15)	0.0065 (14)	−0.0047 (12)	0.0183 (13)
C10	0.0502 (14)	0.0593 (15)	0.0508 (14)	−0.0011 (12)	−0.0094 (12)	0.0054 (11)
C11	0.0356 (12)	0.0519 (13)	0.0398 (12)	−0.0081 (10)	0.0011 (10)	−0.0061 (10)
C12	0.0384 (13)	0.0690 (16)	0.0571 (16)	0.0005 (11)	0.0072 (12)	−0.0090 (12)
C13	0.0431 (15)	0.107 (2)	0.0465 (15)	−0.0073 (16)	0.0091 (12)	−0.0115 (15)
C14	0.0566 (16)	0.101 (2)	0.0409 (14)	−0.0149 (16)	0.0046 (12)	0.0101 (14)
C15	0.0558 (15)	0.0680 (16)	0.0439 (14)	−0.0074 (13)	−0.0002 (12)	0.0093 (11)
C16	0.0421 (12)	0.0479 (12)	0.0353 (11)	−0.0058 (10)	0.0009 (10)	−0.0019 (9)

C17	0.0521 (14)	0.0374 (11)	0.0424 (12)	0.0003 (10)	−0.0031 (10)	0.0038 (9)
C18	0.0752 (18)	0.0435 (13)	0.0511 (14)	0.0196 (12)	0.0162 (13)	0.0044 (11)
C19	0.0484 (14)	0.0637 (15)	0.0493 (14)	0.0162 (12)	0.0058 (11)	−0.0034 (12)
C20	0.0558 (15)	0.0395 (12)	0.0426 (13)	−0.0031 (11)	0.0082 (11)	−0.0034 (9)
N1	0.0394 (10)	0.0391 (10)	0.0390 (10)	0.0013 (8)	−0.0002 (8)	0.0034 (7)
N2	0.0388 (10)	0.0402 (10)	0.0368 (9)	0.0005 (8)	−0.0002 (8)	−0.0001 (7)
N3	0.0464 (11)	0.0356 (9)	0.0372 (10)	0.0031 (8)	0.0017 (8)	−0.0008 (7)
O1	0.0432 (9)	0.0496 (9)	0.0561 (10)	0.0093 (7)	0.0124 (8)	0.0095 (7)
O2	0.0693 (12)	0.0632 (10)	0.0374 (9)	0.0224 (9)	0.0069 (8)	0.0048 (7)
O3	0.0732 (13)	0.0702 (13)	0.0526 (11)	0.0028 (10)	0.0231 (10)	0.0038 (9)
O4	0.0858 (18)	0.0991 (18)	0.116 (2)	0.0421 (15)	−0.0096 (16)	−0.0057 (16)
O5	0.097 (2)	0.189 (4)	0.104 (2)	−0.011 (2)	−0.0175 (18)	0.046 (2)

Geometric parameters (Å, °)

Cu1—O1	1.9475 (16)	C11—C16	1.412 (3)
Cu1—N3	1.9492 (17)	C11—C12	1.417 (3)
Cu1—O2	1.9715 (17)	C12—C13	1.373 (4)
Cu1—N1	2.0261 (17)	C12—H12	0.93
Cu1—N2	2.2429 (17)	C13—C14	1.377 (4)
C1—N2	1.332 (3)	C13—H13	0.93
C1—C2	1.373 (3)	C14—C15	1.358 (4)
C1—H1	0.93	C14—H14	0.93
C2—C3	1.368 (4)	C15—C16	1.412 (3)
C2—H2	0.93	C15—H15	0.93
C3—C4	1.372 (4)	C16—C17	1.430 (3)
C3—H3	0.93	C17—N3	1.284 (3)
C4—C5	1.385 (3)	C17—H17	0.93
C4—H4	0.93	C18—N3	1.473 (3)
C5—N2	1.344 (3)	C18—C19	1.507 (3)
C5—C6	1.486 (3)	C18—H18A	0.97
C6—N1	1.341 (3)	C18—H18B	0.97
C6—C7	1.388 (3)	C19—C20	1.503 (3)
C7—C8	1.374 (4)	C19—H19A	0.97
C7—H7	0.93	C19—H19B	0.97
C8—C9	1.359 (4)	C20—O3	1.231 (3)
C8—H8	0.93	C20—O2	1.279 (3)
C9—C10	1.376 (3)	O4—H4A	0.842 (10)
C9—H9	0.93	O4—H4B	0.847 (10)
C10—N1	1.334 (3)	O5—H5B	0.842 (10)
C10—H10	0.93	O5—H5A	0.822 (10)
C11—O1	1.311 (3)		
O1—Cu1—N3	92.45 (7)	C11—C12—H12	119.3
O1—Cu1—O2	158.33 (8)	C12—C13—C14	121.4 (3)
N3—Cu1—O2	92.82 (7)	C12—C13—H13	119.3
O1—Cu1—N1	87.53 (7)	C14—C13—H13	119.3
N3—Cu1—N1	176.87 (7)	C15—C14—C13	118.9 (3)
O2—Cu1—N1	86.08 (7)	C15—C14—H14	120.6
O1—Cu1—N2	94.25 (7)	C13—C14—H14	120.6

N3—Cu1—N2	105.81 (7)	C14—C15—C16	121.8 (3)
O2—Cu1—N2	104.48 (7)	C14—C15—H15	119.1
N1—Cu1—N2	77.31 (7)	C16—C15—H15	119.1
N2—C1—C2	123.2 (2)	C11—C16—C15	119.7 (2)
N2—C1—H1	118.4	C11—C16—C17	122.9 (2)
C2—C1—H1	118.4	C15—C16—C17	117.4 (2)
C3—C2—C1	118.0 (2)	N3—C17—C16	127.3 (2)
C3—C2—H2	121.0	N3—C17—H17	116.3
C1—C2—H2	121.0	C16—C17—H17	116.3
C2—C3—C4	120.1 (2)	N3—C18—C19	112.96 (19)
C2—C3—H3	120.0	N3—C18—H18A	109.0
C4—C3—H3	120.0	C19—C18—H18A	109.0
C3—C4—C5	118.9 (2)	N3—C18—H18B	109.0
C3—C4—H4	120.5	C19—C18—H18B	109.0
C5—C4—H4	120.5	H18A—C18—H18B	107.8
N2—C5—C4	121.2 (2)	C20—C19—C18	113.1 (2)
N2—C5—C6	115.90 (17)	C20—C19—H19A	109.0
C4—C5—C6	122.85 (19)	C18—C19—H19A	109.0
N1—C6—C7	120.4 (2)	C20—C19—H19B	109.0
N1—C6—C5	116.53 (17)	C18—C19—H19B	109.0
C7—C6—C5	123.0 (2)	H19A—C19—H19B	107.8
C8—C7—C6	119.7 (2)	O3—C20—O2	123.2 (2)
C8—C7—H7	120.1	O3—C20—C19	120.0 (2)
C6—C7—H7	120.1	O2—C20—C19	116.8 (2)
C9—C8—C7	119.4 (2)	C10—N1—C6	118.93 (19)
C9—C8—H8	120.3	C10—N1—Cu1	122.66 (15)
C7—C8—H8	120.3	C6—N1—Cu1	118.33 (14)
C8—C9—C10	118.5 (2)	C1—N2—C5	118.58 (19)
C8—C9—H9	120.8	C1—N2—Cu1	129.79 (15)
C10—C9—H9	120.8	C5—N2—Cu1	111.28 (13)
N1—C10—C9	122.9 (2)	C17—N3—C18	116.33 (18)
N1—C10—H10	118.5	C17—N3—Cu1	125.17 (15)
C9—C10—H10	118.5	C18—N3—Cu1	118.45 (14)
O1—C11—C16	123.7 (2)	C11—O1—Cu1	127.19 (14)
O1—C11—C12	119.6 (2)	C20—O2—Cu1	125.81 (15)
C16—C11—C12	116.7 (2)	H4A—O4—H4B	107 (2)
C13—C12—C11	121.4 (3)	H5B—O5—H5A	108 (2)
C13—C12—H12	119.3		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4A···O2^{i}	0.842 (10)	2.34 (3)	3.075 (4)	146 (5)
O4—H4B···O1	0.847 (10)	1.96 (1)	2.801 (3)	174 (3)
O5—H5B···O3	0.842 (10)	1.99 (2)	2.794 (4)	160 (5)

Symmetry codes: (i) −*x*+1/2, −*y*+3/2, −*z*+1.

Fig. 1

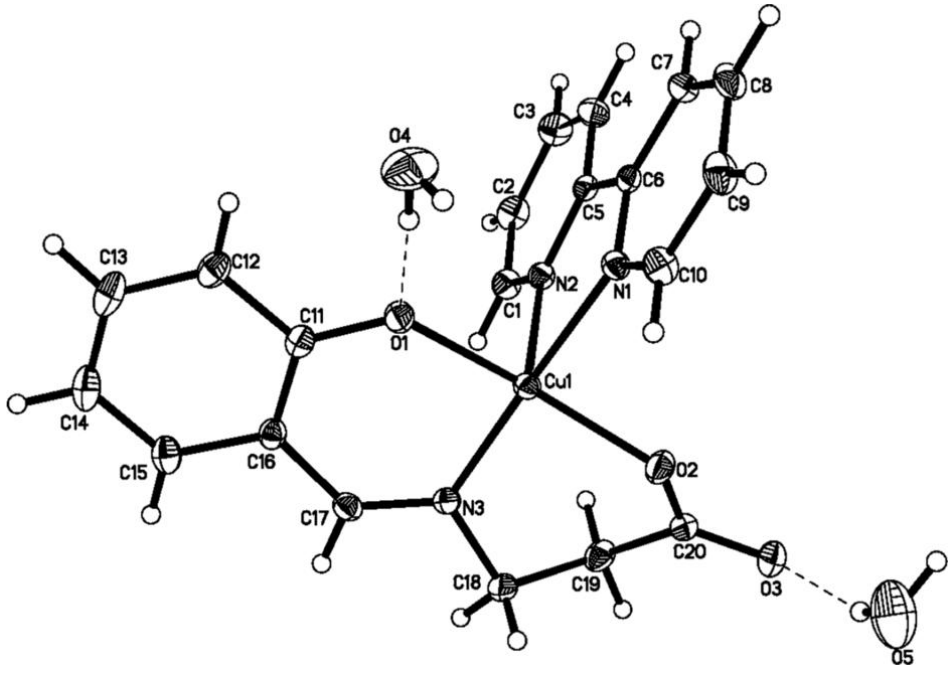
C7
C8
C3
C4
O4
C2
C6
C5
C9
C13
C12
C1
N2
N1
C10
C11
O1
Cu1
C14
C15
C16
O2
C17
N3
C20
C18
C19
O3
O5

Fig. 2