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{3-[Bis(2-pyridylmethyl-κ*N*)amino-κ*N*]-propanol}bis(nitrato-κ*O*)copper(II)

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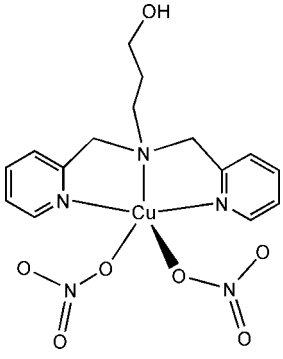
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.006 Å; R factor = 0.053; wR factor = 0.151; data-to-parameter ratio = 17.4.

In the title compound, $[Cu(NO_3)_2(C_{15}H_{19}N_3O)]$, the Cu^{II} ion is coordinated by the N atoms of the tetradentate 3-[bis(2-pyridylmethyl)amino]propanol ligand and two O atoms from two monodentate nitrate anions, resulting in a distorted square-pyramidal environment. An intermolecular O—H···O hydrogen-bonding interaction between the free hydroxy group of the ligand and a nitrate O atom of an adjacent complex unit, gives a chain structure which extends across the (101) planes.

Related literature

Polyamine complexes have been characterized in order to elucidate the mechanisms of metalloenzymes, see: Tshuva & Lippard (2004). For complexes with bis(2-pyridylmethyl)-amine ligands, see: Bebout *et al.* (1998); Shin *et al.* (2010). Compounds with tridentate units have potential biological applications, see: van Staveren *et al.* (2002). Palladium(II) and platinum(II) complexes with bis(2-pyridylmethyl)amine or its derivatives have been investigated as potential anticancer agents including *cis*-platin (Rauterkus *et al.*, 2003). For the preparation of *N*,*N*-bis(2-pyridylmethyl)-3-aminopropanol, see: Young *et al.* (1995).



Experimental

Crystal data

$[Cu(NO_3)_2(C_{15}H_{19}N_3O)]$
M_r = 444.89
Monoclinic, $P2_1/n$
a = 8.3499 (7) Å
b = 14.7703 (12) Å
c = 14.5134 (12) Å
β = 95.055 (2)°
V = 1783.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.28 mm^{-1}
T = 200 K
0.26 × 0.13 × 0.09 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.820, T_{max} = 0.892
13134 measured reflections
4412 independent reflections
2297 reflections with $I > 2\sigma(I)$
R_{int} = 0.078

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.151
S = 1.04
4412 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O7^{i}	0.84	2.18	2.961 (6)	155

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2083).

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supplementary materials

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{3-[Bis(2-pyridylmethyl-*κN*)amino-*κN*]propanol}bis(nitrato-*κO*)copper(II)

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Comment

The preparation and characterization of a large number of polyamine complexes has been done, in order to elucidate the mechanisms of metalloenzymes (Tshuva & Lippard, 2004). Recently, the complexes with bis(2-pyridylmethyl)amine moieties have been widely described (Bebout *et al.*,1998; Shin *et al.*, 2010) because the tridentate unit is a good candidate for potential biological applications (van Staveren *et al.*, 2002). For example, palladium(II) and platinum(II) complexes with bis(2-pyridylmethyl)amine or its derivatives have been investigated as potential anticancer agents, e.g. *cis*-platin (Rauterkus *et al.*, 2003). Here, we report the synthesis and crystal structure of five-coordinate $Cu(NO_3)_2$ complex with the tetradentate ligand *N*,*N*-bis(2-pyridylmethyl)-3-aminopropanol = bdap), the title compound [Cu(bpap)$(NO_3)_2$] (I), and the structure is reported here.

In the title compound (Fig. 1), the Cu^{II} ion is five-coordinated and exhibits a distorted square pyramidal geometry, the equatorial plane being defined by the three nitrogen atoms of the bdap ligand and one oxygen atom of a nitrate ion. The coordination geometry is completed by the axial coordination of the oxygen atom of the second nitrate anion. The Cu—L_{eq} bond lengths are in the range of 1.965 (4) and 2.093 (3) Å and the Cu—O_{ax} bond length is 2.248 (3) Å. Both nitrate ions are bound in η^1-fashion. The bond angles about the copper atom range from 76.95 (12) to 165.48 (15)°. The packing structure involves a strong O—H···O hydrogen bonding interaction between the free hydroxyl group of the bpap ligand and a nitrate O atom of an adjacent complex unit (Table 1), giving a one-dimensional chain structure which extends across the (101) planes in the unit cell (Fig. 2).

Experimental

A MeOH solution (5 ml) of $Cu(NO_3)_2$. $3H_2O$ (47 mg, 0.194 mmol) was added to a MeOH solution (5 ml) of *N*,*N*-bis(2-pyridylmethyl)-3-aminopropanol (bpap, 50 mg, 0.194 mmol) (Young *et al.*, 1995). The color changed to blue-green, and the solution was stirred for 10 min at room temperature. Blue-green crystals were obtained by diffusion of diethyl ether into the reaction mixture in methanol and were collected by filtration, washed with diethyl ether, and dried in air (yield: 36 mg, 42%). FTIR (KBr, cm^{-1}): 3399, 1437, 3069, 2970, 2862, 1054, 1608.

Refinement

All H atoms in the title compound were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (ring H atoms) or 0.99 (open chain H atoms) Å and an O—H distance of 0.84 Å, and with U_{iso}(H) values of 1.2 or 1.5 times U_{eq}(C,O).

Figures

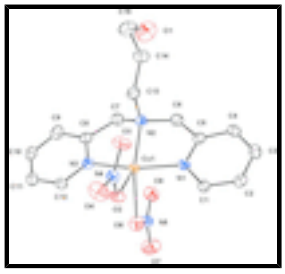

Fig. 1. *ORTEP* drawing of the title compound with atomic numbering scheme and 30% probability ellipsoids.

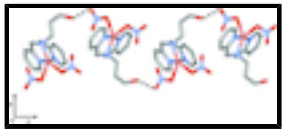

Fig. 2. A view of the title compound showing a one-dimensional chain structure formed by O—H···O hydrogen-bonding interactions.

{3-[Bis(2-pyridylmethyl-κ*N*)amino-κ*N*]propanol}bis(nitrato- κ*O*)copper(II)

Crystal data

$[Cu(NO_3)_2(C_{15}H_{19}N_3O)]$	$F(000) = 916$
$M_r = 444.89$	$D_x = 1.657$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2504 reflections
$a = 8.3499$ (7) Å	$\theta = 2.7$–$23.6°$
$b = 14.7703$ (12) Å	$\mu = 1.28$ mm^{-1}
$c = 14.5134$ (12) Å	$T = 200$ K
$\beta = 95.055$ (2)°	Needle, blue-green
$V = 1783.0$ (3) Å^3	0.26 × 0.13 × 0.09 mm
$Z = 4$	

Data collection

Siemens SMART CCD diffractometer	4412 independent reflections
Radiation source: fine-focus sealed tube	2297 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.078$
φ and ω scans	$\theta_{max} = 28.3°$, $\theta_{min} = 2.0°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.820$, $T_{max} = 0.892$	$k = -19 \rightarrow 18$
13134 measured reflections	$l = -17 \rightarrow 19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.053$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.151$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
4412 reflections	$(\Delta/\sigma)_{max} < 0.001$
254 parameters	$\Delta\rho_{max} = 0.78$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.66$ e Å^{-3}

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	0.13958 (6)	0.34362 (4)	0.87320 (4)	0.03228 (19)
N1	−0.0717 (4)	0.3222 (2)	0.9189 (2)	0.0314 (9)
N2	0.1137 (4)	0.2127 (2)	0.8271 (2)	0.0336 (9)
N3	0.3346 (4)	0.3396 (2)	0.8064 (2)	0.0320 (8)
N4	0.2941 (4)	0.3812 (3)	1.0535 (2)	0.0344 (9)

N5	0.0028 (5)	0.4753 (3)	0.7451 (3)	0.0464 (11)
O1	0.2165 (5)	0.0185 (3)	1.0483 (3)	0.0818 (13)
H1	0.2959	0.0168	1.0880	0.123*
O2	0.2405 (4)	0.4250 (2)	0.9813 (2)	0.0396 (8)
O3	0.2729 (4)	0.2988 (2)	1.0556 (2)	0.0539 (10)
O4	0.3673 (4)	0.4229 (3)	1.1171 (2)	0.0614 (11)
O5	0.0804 (4)	0.4846 (2)	0.8229 (2)	0.0497 (9)
O6	−0.0202 (4)	0.3980 (3)	0.7120 (2)	0.0598 (10)
O7	−0.0504 (5)	0.5423 (3)	0.7013 (3)	0.0789 (13)
C1	−0.1437 (5)	0.3745 (3)	0.9779 (3)	0.0323 (10)
H1A	−0.0927	0.4290	0.9992	0.039*
C2	−0.2890 (5)	0.3519 (3)	1.0086 (3)	0.0373 (11)
H2	−0.3394	0.3908	1.0496	0.045*
C3	−0.3605 (6)	0.2721 (3)	0.9791 (3)	0.0401 (12)
H3	−0.4592	0.2541	1.0015	0.048*
C4	−0.2894 (5)	0.2181 (3)	0.9172 (3)	0.0382 (11)
H4	−0.3384	0.1630	0.8957	0.046*
C5	−0.1448 (5)	0.2458 (3)	0.8868 (3)	0.0335 (10)
C6	−0.0626 (6)	0.1966 (3)	0.8132 (3)	0.0410 (12)
H6A	−0.0849	0.1309	0.8165	0.049*
H6B	−0.1046	0.2186	0.7513	0.049*
C7	0.1975 (6)	0.2068 (3)	0.7424 (3)	0.0427 (12)
H7A	0.1229	0.2238	0.6884	0.051*
H7B	0.2328	0.1436	0.7336	0.051*
C8	0.3421 (5)	0.2690 (3)	0.7485 (3)	0.0361 (11)
C9	0.4694 (6)	0.2583 (3)	0.6956 (3)	0.0451 (13)
H9	0.4763	0.2069	0.6569	0.054*
C10	0.5875 (6)	0.3244 (3)	0.7002 (3)	0.0427 (12)
H10	0.6751	0.3195	0.6629	0.051*
C11	0.5779 (6)	0.3969 (3)	0.7584 (3)	0.0404 (11)
H11	0.6579	0.4427	0.7616	0.049*
C12	0.4513 (5)	0.4020 (3)	0.8115 (3)	0.0341 (10)
H12	0.4458	0.4512	0.8532	0.041*
C13	0.1911 (6)	0.1521 (3)	0.9023 (3)	0.0402 (11)
H13A	0.1480	0.1690	0.9613	0.048*
H13B	0.3079	0.1650	0.9089	0.048*
C14	0.1684 (6)	0.0503 (3)	0.8885 (4)	0.0543 (14)
H14A	0.0536	0.0348	0.8910	0.065*
H14B	0.2000	0.0331	0.8267	0.065*
C15	0.2670 (8)	−0.0015 (4)	0.9608 (4)	0.0659 (17)
H15A	0.2553	−0.0672	0.9485	0.079*
H15B	0.3818	0.0147	0.9594	0.079*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0363 (3)	0.0263 (3)	0.0347 (3)	−0.0016 (2)	0.0056 (2)	−0.0041 (2)
N1	0.034 (2)	0.026 (2)	0.034 (2)	−0.0022 (16)	0.0002 (17)	−0.0023 (15)

N2	0.035 (2)	0.033 (2)	0.032 (2)	−0.0039 (17)	0.0023 (17)	−0.0098 (16)
N3	0.033 (2)	0.033 (2)	0.030 (2)	0.0007 (17)	0.0041 (16)	0.0008 (16)
N4	0.037 (2)	0.037 (2)	0.030 (2)	−0.0022 (18)	0.0066 (18)	−0.0032 (18)
N5	0.047 (3)	0.039 (3)	0.054 (3)	0.004 (2)	0.007 (2)	0.010 (2)
O1	0.091 (3)	0.092 (4)	0.063 (3)	0.022 (3)	0.010 (2)	0.003 (2)
O2	0.054 (2)	0.0318 (19)	0.0322 (18)	−0.0032 (15)	0.0001 (15)	−0.0030 (14)
O3	0.073 (3)	0.030 (2)	0.056 (2)	−0.0080 (18)	−0.0066 (19)	0.0031 (17)
O4	0.082 (3)	0.062 (3)	0.037 (2)	−0.020 (2)	−0.0132 (19)	−0.0105 (17)
O5	0.055 (2)	0.053 (2)	0.040 (2)	0.0027 (17)	−0.0047 (18)	0.0028 (16)
O6	0.061 (2)	0.058 (3)	0.059 (2)	−0.009 (2)	0.0001 (19)	−0.001 (2)
O7	0.099 (3)	0.065 (3)	0.070 (3)	0.025 (2)	−0.006 (2)	0.034 (2)
C1	0.033 (3)	0.032 (3)	0.032 (2)	−0.0024 (19)	0.007 (2)	−0.0065 (19)
C2	0.041 (3)	0.036 (3)	0.035 (3)	0.006 (2)	0.002 (2)	−0.003 (2)
C3	0.037 (3)	0.048 (3)	0.036 (3)	−0.003 (2)	0.005 (2)	0.004 (2)
C4	0.042 (3)	0.031 (3)	0.040 (3)	−0.006 (2)	−0.003 (2)	−0.001 (2)
C5	0.035 (3)	0.033 (3)	0.032 (2)	0.003 (2)	0.000 (2)	0.0013 (19)
C6	0.041 (3)	0.036 (3)	0.045 (3)	−0.002 (2)	−0.004 (2)	−0.010 (2)
C7	0.046 (3)	0.039 (3)	0.043 (3)	−0.005 (2)	0.005 (2)	−0.012 (2)
C8	0.042 (3)	0.033 (3)	0.033 (3)	0.003 (2)	0.003 (2)	−0.004 (2)
C9	0.046 (3)	0.052 (3)	0.037 (3)	0.005 (3)	0.007 (2)	−0.012 (2)
C10	0.032 (3)	0.055 (4)	0.042 (3)	0.004 (2)	0.008 (2)	0.001 (2)
C11	0.037 (3)	0.046 (3)	0.038 (3)	0.001 (2)	0.003 (2)	0.006 (2)
C12	0.039 (3)	0.028 (3)	0.034 (3)	−0.002 (2)	−0.001 (2)	0.0002 (19)
C13	0.040 (3)	0.034 (3)	0.046 (3)	0.004 (2)	−0.002 (2)	−0.004 (2)
C14	0.066 (4)	0.038 (3)	0.059 (3)	0.001 (3)	0.004 (3)	−0.002 (2)
C15	0.091 (5)	0.055 (4)	0.053 (4)	0.021 (3)	0.015 (3)	0.008 (3)

Geometric parameters (Å, °)

Cu1—N1	1.965 (4)	C3—H3	0.9500
Cu1—N3	1.968 (3)	C4—C5	1.383 (6)
Cu1—N2	2.051 (3)	C4—H4	0.9500
Cu1—O2	2.093 (3)	C5—C6	1.507 (6)
Cu1—O5	2.248 (3)	C6—H6A	0.9900
N1—C1	1.335 (5)	C6—H6B	0.9900
N1—C5	1.345 (5)	C7—C8	1.514 (6)
N2—C7	1.469 (5)	C7—H7A	0.9900
N2—C6	1.487 (5)	C7—H7B	0.9900
N2—C13	1.512 (6)	C8—C9	1.374 (6)
N3—C12	1.339 (5)	C9—C10	1.385 (6)
N3—C8	1.343 (5)	C9—H9	0.9500
N4—O4	1.227 (4)	C10—C11	1.370 (6)
N4—O3	1.230 (4)	C10—H10	0.9500
N4—O2	1.279 (4)	C11—C12	1.364 (6)
N5—O7	1.236 (5)	C11—H11	0.9500
N5—O6	1.247 (5)	C12—H12	0.9500
N5—O5	1.259 (5)	C13—C14	1.527 (6)
O1—C15	1.403 (6)	C13—H13A	0.9900
O1—H1	0.8400	C13—H13B	0.9900

C1—C2	1.370 (6)	C14—C15	1.487 (7)
C1—H1A	0.9500	C14—H14A	0.9900
C2—C3	1.373 (6)	C14—H14B	0.9900
C2—H2	0.9500	C15—H15A	0.9900
C3—C4	1.375 (6)	C15—H15B	0.9900
N1—Cu1—N3	165.48 (15)	N2—C6—C5	109.5 (4)
N1—Cu1—N2	83.45 (14)	N2—C6—H6A	109.8
N3—Cu1—N2	83.03 (14)	C5—C6—H6A	109.8
N1—Cu1—O2	98.85 (13)	N2—C6—H6B	109.8
N3—Cu1—O2	95.20 (13)	C5—C6—H6B	109.8
N2—Cu1—O2	144.03 (14)	H6A—C6—H6B	108.2
N1—Cu1—O5	94.64 (13)	N2—C7—C8	110.6 (4)
N3—Cu1—O5	92.06 (14)	N2—C7—H7A	109.5
N2—Cu1—O5	138.91 (14)	C8—C7—H7A	109.5
O2—Cu1—O5	76.95 (12)	N2—C7—H7B	109.5
C1—N1—C5	119.4 (4)	C8—C7—H7B	109.5
C1—N1—Cu1	126.3 (3)	H7A—C7—H7B	108.1
C5—N1—Cu1	114.3 (3)	N3—C8—C9	121.3 (4)
C7—N2—C6	114.5 (4)	N3—C8—C7	115.2 (4)
C7—N2—C13	111.3 (4)	C9—C8—C7	123.4 (4)
C6—N2—C13	111.0 (3)	C8—C9—C10	118.4 (4)
C7—N2—Cu1	106.5 (3)	C8—C9—H9	120.8
C6—N2—Cu1	105.6 (3)	C10—C9—H9	120.8
C13—N2—Cu1	107.2 (3)	C11—C10—C9	120.0 (4)
C12—N3—C8	119.6 (4)	C11—C10—H10	120.0
C12—N3—Cu1	125.6 (3)	C9—C10—H10	120.0
C8—N3—Cu1	114.7 (3)	C12—C11—C10	118.8 (5)
O4—N4—O3	122.8 (4)	C12—C11—H11	120.6
O4—N4—O2	118.5 (4)	C10—C11—H11	120.6
O3—N4—O2	118.6 (4)	N3—C12—C11	121.8 (4)
O7—N5—O6	119.9 (5)	N3—C12—H12	119.1
O7—N5—O5	120.4 (5)	C11—C12—H12	119.1
O6—N5—O5	119.7 (4)	N2—C13—C14	116.6 (4)
C15—O1—H1	109.5	N2—C13—H13A	108.1
N4—O2—Cu1	114.4 (3)	C14—C13—H13A	108.1
N5—O5—Cu1	105.7 (3)	N2—C13—H13B	108.1
N1—C1—C2	122.0 (4)	C14—C13—H13B	108.1
N1—C1—H1A	119.0	H13A—C13—H13B	107.3
C2—C1—H1A	119.0	C15—C14—C13	111.1 (4)
C1—C2—C3	118.7 (4)	C15—C14—H14A	109.4
C1—C2—H2	120.7	C13—C14—H14A	109.4
C3—C2—H2	120.7	C15—C14—H14B	109.4
C2—C3—C4	120.1 (4)	C13—C14—H14B	109.4
C2—C3—H3	119.9	H14A—C14—H14B	108.0
C4—C3—H3	119.9	O1—C15—C14	109.8 (5)
C3—C4—C5	118.4 (4)	O1—C15—H15A	109.7
C3—C4—H4	120.8	C14—C15—H15A	109.7
C5—C4—H4	120.8	O1—C15—H15B	109.7
N1—C5—C4	121.4 (4)	C14—C15—H15B	109.7

N1—C5—C6	115.4 (4)	H15A—C15—H15B	108.2
C4—C5—C6	123.2 (4)		
N3—Cu1—N1—C1	−171.0 (5)	O2—Cu1—O5—N5	−179.4 (3)
N2—Cu1—N1—C1	167.4 (4)	C5—N1—C1—C2	1.4 (6)
O2—Cu1—N1—C1	23.7 (4)	Cu1—N1—C1—C2	−177.4 (3)
O5—Cu1—N1—C1	−53.8 (4)	N1—C1—C2—C3	1.4 (7)
N3—Cu1—N1—C5	10.1 (8)	C1—C2—C3—C4	−2.4 (7)
N2—Cu1—N1—C5	−11.4 (3)	C2—C3—C4—C5	0.8 (7)
O2—Cu1—N1—C5	−155.2 (3)	C1—N1—C5—C4	−3.2 (6)
O5—Cu1—N1—C5	127.4 (3)	Cu1—N1—C5—C4	175.8 (3)
N1—Cu1—N2—C7	148.6 (3)	C1—N1—C5—C6	173.8 (4)
N3—Cu1—N2—C7	−26.0 (3)	Cu1—N1—C5—C6	−7.3 (5)
O2—Cu1—N2—C7	−115.3 (3)	C3—C4—C5—N1	2.1 (7)
O5—Cu1—N2—C7	59.1 (4)	C3—C4—C5—C6	−174.6 (4)
N1—Cu1—N2—C6	26.4 (3)	C7—N2—C6—C5	−152.9 (4)
N3—Cu1—N2—C6	−148.3 (3)	C13—N2—C6—C5	79.9 (4)
O2—Cu1—N2—C6	122.5 (3)	Cu1—N2—C6—C5	−36.0 (4)
O5—Cu1—N2—C6	−63.1 (3)	N1—C5—C6—N2	30.1 (5)
N1—Cu1—N2—C13	−92.1 (3)	C4—C5—C6—N2	−153.0 (4)
N3—Cu1—N2—C13	93.3 (3)	C6—N2—C7—C8	149.5 (4)
O2—Cu1—N2—C13	4.0 (4)	C13—N2—C7—C8	−83.5 (4)
O5—Cu1—N2—C13	178.4 (2)	Cu1—N2—C7—C8	33.1 (4)
N1—Cu1—N3—C12	169.3 (5)	C12—N3—C8—C9	1.5 (6)
N2—Cu1—N3—C12	−169.2 (4)	Cu1—N3—C8—C9	178.5 (3)
O2—Cu1—N3—C12	−25.3 (4)	C12—N3—C8—C7	−175.2 (4)
O5—Cu1—N3—C12	51.7 (3)	Cu1—N3—C8—C7	1.8 (5)
N1—Cu1—N3—C8	−7.5 (8)	N2—C7—C8—N3	−24.4 (6)
N2—Cu1—N3—C8	14.0 (3)	N2—C7—C8—C9	159.0 (4)
O2—Cu1—N3—C8	157.9 (3)	N3—C8—C9—C10	−2.8 (7)
O5—Cu1—N3—C8	−125.0 (3)	C7—C8—C9—C10	173.6 (4)
O4—N4—O2—Cu1	173.9 (3)	C8—C9—C10—C11	1.8 (7)
O3—N4—O2—Cu1	−4.6 (5)	C9—C10—C11—C12	0.4 (7)
N1—Cu1—O2—N4	79.6 (3)	C8—N3—C12—C11	0.8 (6)
N3—Cu1—O2—N4	−96.7 (3)	Cu1—N3—C12—C11	−175.8 (3)
N2—Cu1—O2—N4	−11.4 (4)	C10—C11—C12—N3	−1.8 (7)
O5—Cu1—O2—N4	172.4 (3)	C7—N2—C13—C14	−71.2 (5)
O7—N5—O5—Cu1	177.9 (4)	C6—N2—C13—C14	57.7 (5)
O6—N5—O5—Cu1	−2.2 (5)	Cu1—N2—C13—C14	172.7 (3)
N1—Cu1—O5—N5	−81.4 (3)	N2—C13—C14—C15	172.9 (4)
N3—Cu1—O5—N5	85.7 (3)	C13—C14—C15—O1	62.6 (6)
N2—Cu1—O5—N5	3.9 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O7^{i}	0.84	2.18	2.961 (6)	155

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

Fig. 1

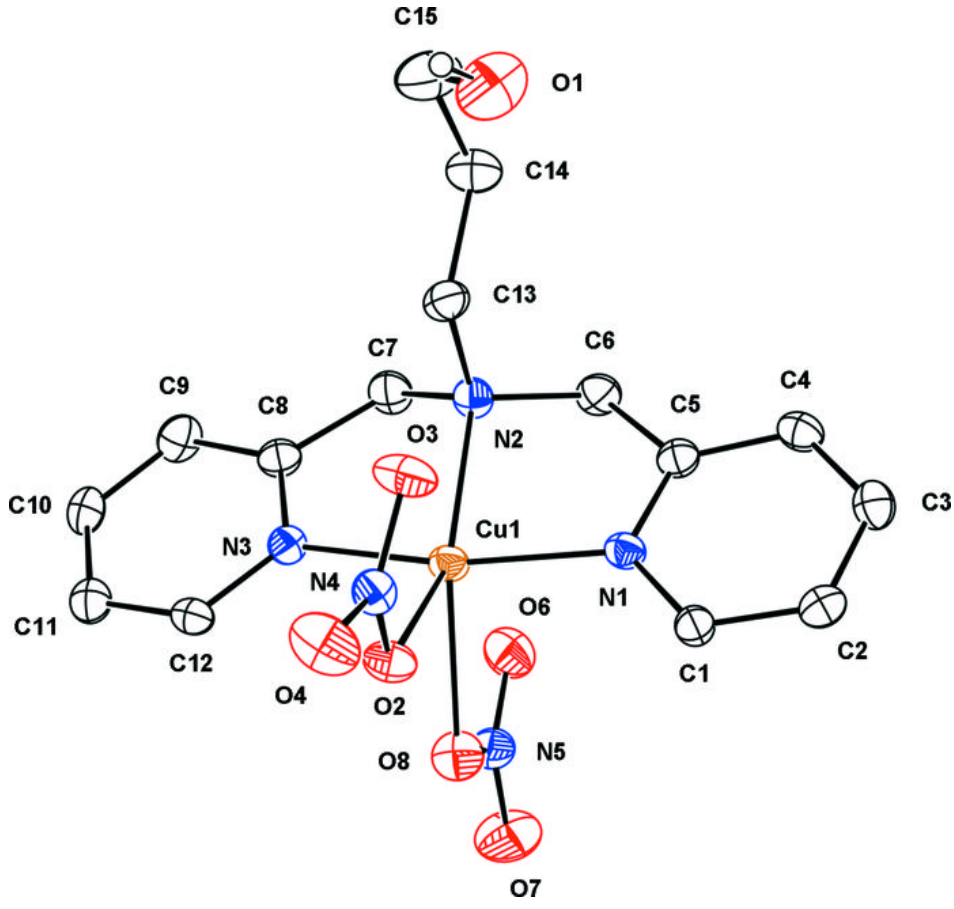
C15
O1
C14
C13
C7
C6
C9
C8
C4
C5
O3
N2
C10
C3
Cu1
N3
N4
N1
O6
C11
C12
C2
C1
O4
O2
O8
N5
O7

Fig. 2