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Acetonitrile{3-[bis(2-pyridylmethyl-κN)-amino-κN]propanol-κO}(perchlorato-κO)copper(II) perchlorate

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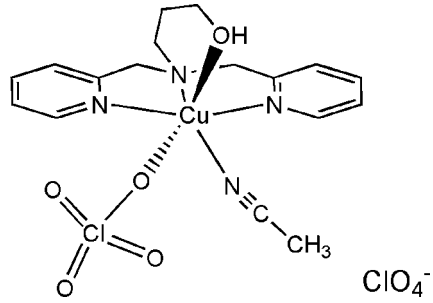
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.008 Å; R factor = 0.061; wR factor = 0.188; data-to-parameter ratio = 18.5.

In the title compound, $[Cu(ClO_4)(C_2H_3N)(C_{15}H_{19}N_3O)]ClO_4$, the Cu^{II} ion is coordinated by three N atoms and a hydroxyl-O atom of the tetradentate ligand, an O atom of a perchlorate ion and an N atom of an acetonitrile ligand giving a tetragonally distorted octahedral environment around the copper(II) atom. There is an offset inter-complex face-to-face π–π interaction [centroid–centroid distance = 3.718 (2) Å] involving one of the pyridine rings of the ligand as well as an intra-complex O—H···O hydrogen-bonding interaction between the coordinated hydroxyl group of the ligand and the perchlorate counter-ion.

Related literature

The preparation and characterization of polyamine complexes have allowed the elucidatation of the mechanisms of metalloenzyme reactions, see: Tshuva & Lippard (2004). For studies of complexes with bis(2-pyridylmethyl)amine moieties, see: Bebout *et al.* (1998); Shin *et al.* (2010). For potential biological applications of the tridentate unit, see: van Staveren *et al.* (2002). Examples include the use of Pd^{II} and Pt^{II} complexes with bis(2-pyridylmethyl)amine or its derivatives as anticancer agents, e.g. *cis*-platin (Rauterkus *et al.*, 2003). For intercomplex π–π stacking interactions, see: Shetty *et al.* (1996). For the preparation of *N*,*N*-bis(2-pyridylmethyl)-3-aminopropanol, see: Young *et al.* (1995).



Experimental

Crystal data

$[Cu(ClO_4)(C_2H_3N)(C_{15}H_{19}N_3O)]ClO_4$
M_r = 560.83
Monoclinic, $C2/c$
a = 18.8394 (16) Å
b = 10.6049 (9) Å
c = 23.171 (2) Å
β = 102.998 (2)°
V = 4510.7 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.26 mm^{-1}
T = 200 K
0.20 × 0.17 × 0.08 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.777, T_{max} = 0.904
16472 measured reflections
5616 independent reflections
3249 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.188
S = 1.11
5616 reflections
303 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.66 e Å^{-3}
$\Delta\rho_{min}$ = −1.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O9	0.74 (5)	2.46 (5)	3.090 (12)	145 (5)

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: ZS2085).

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Acetonitrile{3-[bis(2-pyridylmethyl-*κN*)amino-*κN*]propanol-*κO*}(perchlorato-*κO*)copper(II) perchlorate

Jong Won Shin, Sankara Rao Rowthu, Hyun Jung Cho and Kil Sik Min

S1. Comment

The preparation and characterization of polyamine complexes have allowed the elucidatation of the mechanisms of metalloenzyme reactions (Tshuva & Lippard, 2004). The complexes with bis(2-pyridylmethyl)amine moieties have been widely studied (Bebout *et al.*,1998; Shin *et al.*, 2010) because the tridentate unit has potential in biological applications (van Staveren *et al.*, 2002), examples being the Pd^{II} and Pt^{II} complexes with bis(2-pyridylmethyl)amine or its derivatives, as anticancer agents, e.g. *cis*-platin (Rauterkus *et al.*, 2003). Here, we report the synthesis and crystal structure of a six-coordidine Cu^{II} complex with *N*,*N*-bis(2-pyridylmethyl)-3-aminopropanol (bpapOH), the title compound [Cu(bpapOH)$(CH_3CN)(ClO_4)$] ClO_4 (I).

In the title compound (Fig. 1) the copper(II) ion is bonded to three N atoms of the tetradentate ligand and one N atom from an acetonitrile solvent molecule in an equatorial plane and two O atoms in axial sites, one from the hydroxyl group of the ligand, the other from a perchlorate ion, resulting in a tetragonally distorted octahedral stereochemistry. The bond lengths around Cu^{II} in the equatorial plane are in the range of 1.986 (4)–2.021 (4) Å while the axial Cu–O distances are 2.232 (4) Å (hydroxy) and 2.868 (4) Å (perchlorate), due to Jahn-Teller distortion. The bond angles about the copper atom lie in the range 84.12 (17)–178.30 (19)°. One of the pyridyl groups of the coordinated bpapOH ligand (N1–C5) is involved in a an offset face-to-face *π*–*π* inter-complex stacking interaction (Shetty *et al.*, 1996) (ring centroid separation $Cg1\cdots Cg^{i}$, 3.718 (2) Å], giving dimers (Fig. 2) [symmetry code: (i) -*x* + 1/2, -*y* + 1/2, -*z* + 1]. The inter-planar separation of these pyridine rings is 3.491 (2) Å and the dihedral angle between the pyridine ring planes is 0.0°. Additionally, an intra-complex O—H···O hydrogen-bonding interaction is found between the hydroxyl group of the ligand and the free perchlorate anion (Table 1) (Fig. 3).

S2. Experimental

A MeOH solution (5 ml) of $Cu(ClO_4)_2 \cdot 6H_2O$ (72 mg, 0.194 mmol) was added to a MeOH solution (5 ml) of *N*,*N*-bis(2-pyridylmethyl)-3-aminopropanol (bpapOH) (50 mg, 0.194 mmol) (Young *et al.*, 1995). The mixture was stirred for 10 min at room temperature, resulting in a color change to blue-green. Diffusion of diethylether into the mixture gave blue crystals of the title compound after a few days and these were washed with diethyl ether and dried in air (yield: 43 mg, 40%). FTIR (KBr, cm^{-1}): *ν*(OH), 3393; *ν*(ClO_4^-), 1087, 627; *ν*(C—H), 3070, 2862; *ν*(C—N), 1607.

S3. Refinement

All C-bound 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 Å (ring H atoms) and 0.98–0.99 Å (open chain H atoms), and with U_{iso}(H) values of 1.2 or 1.5U_{iso} of the parent C atoms. The hydroxyl H atom was located in a difference Fourier and its position and U_{iso} value were allowed to refine freely.

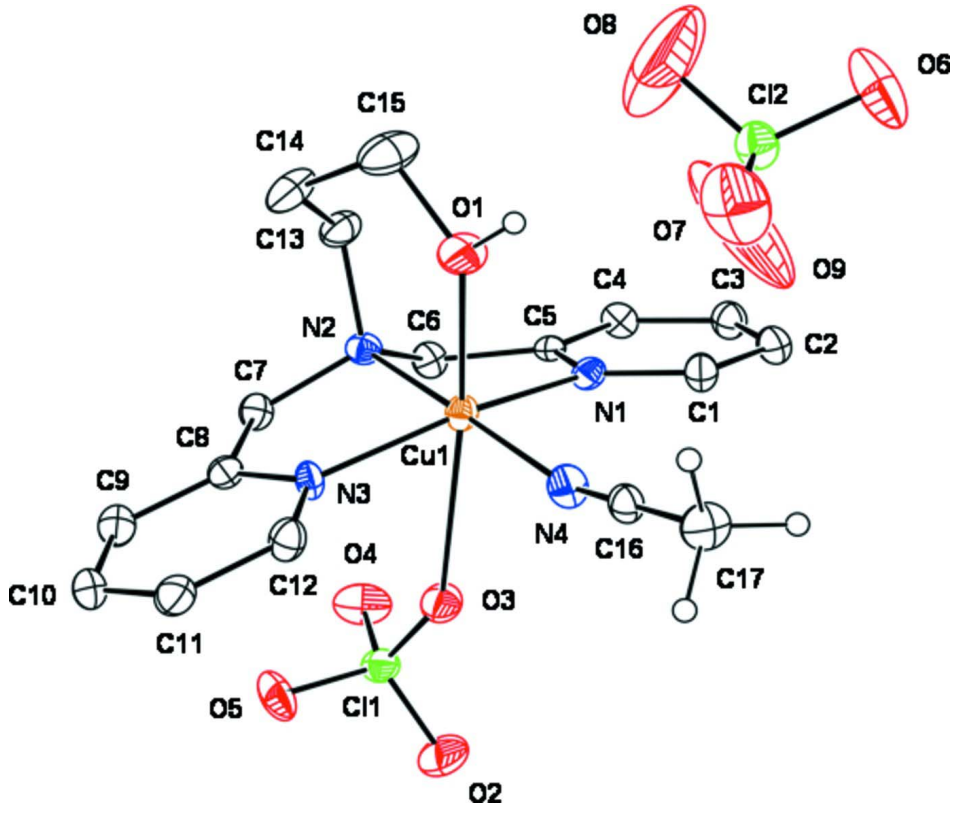

Figure 1

Molecular configuration and atom numbering scheme for the title compound, with 30% probability displacement ellipsoids. Non-H atoms are omitted.

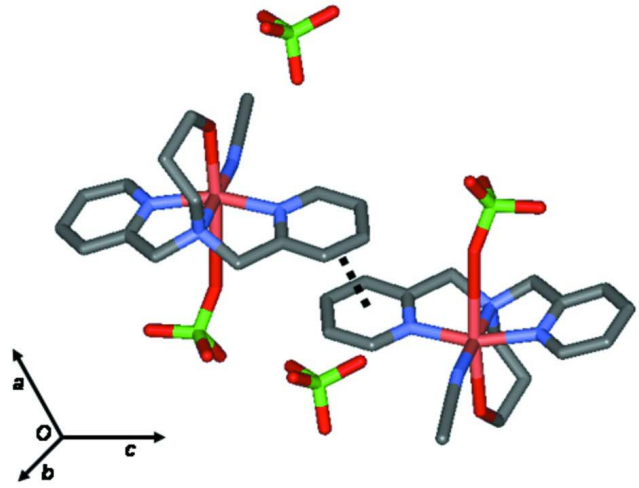

Figure 2

Perspective view of the title compound showing the offset π–π stacking interaction *via* one of the pyridine groups of the ligand, (indicated as a dashed line).

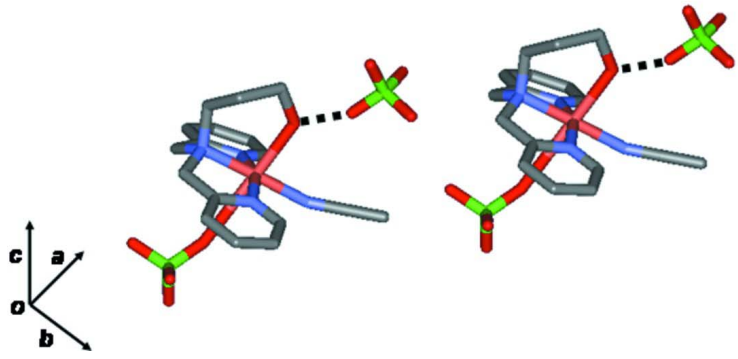

Figure 3

Perspective view of the title compound showing an hydroxyl O—H···O (perchlorate) hydrogen-bonding interaction, indicated as a dashed line.

Acetonitrile{3-[bis(2-pyridylmethyl-*κN*)amino-*κN*]propanol- *κO*}(perchlorato-*κO*)copper(II) perchlorate

Crystal data

$[Cu(ClO_4)(C_2H_3N)(C_{15}H_{19}N_3O)]ClO_4$
M_r = 560.83

Monoclinic, *C*2/*c*
Hall symbol: -C 2yc

a = 18.8394 (16) Å
b = 10.6049 (9) Å
c = 23.171 (2) Å
β = 102.998 (2)°
V = 4510.7 (7) Å^3
Z = 8
F(000) = 2296
D_x = 1.652 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3827 reflections
θ = 2.2–27.2°
μ = 1.26 mm^{-1}
T = 200 K
Block, blue
0.20 × 0.17 × 0.08 mm

Data collection

Siemens SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.777, T_{max} = 0.904

16472 measured reflections
5616 independent reflections
3249 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 28.3°, θ_{min} = 1.8°
h = −25→25
k = −14→14
l = −26→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.188
S = 1.11
5616 reflections
303 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2 + 23.552P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 1.66 e Å^{-3}
$\Delta\rho_{min}$ = −1.16 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	0.13311 (3)	0.19042 (6)	0.63867 (3)	0.0267 (2)
Cl1	0.35845 (8)	0.20097 (13)	0.70690 (6)	0.0348 (3)
Cl2	−0.11763 (8)	0.33890 (14)	0.50981 (7)	0.0397 (4)
N1	0.1499 (2)	0.1811 (4)	0.55716 (19)	0.0263 (9)
N2	0.1661 (2)	0.0086 (4)	0.6439 (2)	0.0279 (10)
N3	0.1492 (2)	0.1799 (4)	0.72643 (18)	0.0266 (9)

N4	0.1036 (3)	0.3717 (4)	0.6338 (2)	0.0352 (11)
O1	0.0140 (2)	0.1484 (4)	0.6184 (2)	0.0464 (12)
H1A	−0.016 (3)	0.176 (5)	0.596 (2)	0.056 (16)*
O2	0.4077 (3)	0.2983 (5)	0.7002 (3)	0.0691 (15)
O3	0.2870 (2)	0.2349 (4)	0.67406 (19)	0.0432 (11)
O4	0.3794 (2)	0.0851 (4)	0.6847 (2)	0.0569 (13)
O5	0.3560 (3)	0.1857 (5)	0.76703 (18)	0.0567 (13)
O6	−0.1520 (3)	0.3725 (7)	0.4524 (2)	0.085 (2)
O7	−0.1319 (4)	0.4221 (6)	0.5530 (3)	0.092 (2)
O8	−0.1411 (9)	0.2274 (8)	0.5240 (4)	0.247 (8)
O9	−0.0464 (4)	0.3278 (15)	0.5138 (3)	0.230 (7)
C1	0.1296 (3)	0.2643 (5)	0.5134 (2)	0.0325 (12)
H1	0.1038	0.3377	0.5203	0.039*
C2	0.1449 (3)	0.2472 (6)	0.4586 (3)	0.0367 (13)
H2	0.1300	0.3076	0.4280	0.044*
C3	0.1825 (3)	0.1403 (5)	0.4491 (3)	0.0362 (13)
H3	0.1942	0.1269	0.4117	0.043*
C4	0.2031 (3)	0.0532 (5)	0.4936 (2)	0.0339 (13)
H4	0.2278	−0.0218	0.4872	0.041*
C5	0.1870 (3)	0.0769 (5)	0.5481 (2)	0.0254 (11)
C6	0.2135 (3)	−0.0071 (5)	0.6006 (2)	0.0314 (12)
H6A	0.2124	−0.0961	0.5876	0.038*
H6B	0.2644	0.0147	0.6198	0.038*
C7	0.2068 (3)	−0.0160 (5)	0.7060 (2)	0.0296 (12)
H7A	0.2598	−0.0110	0.7080	0.035*
H7B	0.1958	−0.1024	0.7176	0.035*
C8	0.1873 (3)	0.0770 (5)	0.7490 (2)	0.0288 (12)
C9	0.2105 (3)	0.0616 (6)	0.8098 (3)	0.0370 (13)
H9	0.2383	−0.0101	0.8257	0.044*
C10	0.1923 (3)	0.1526 (6)	0.8468 (3)	0.0402 (15)
H10	0.2082	0.1449	0.8886	0.048*
C11	0.1511 (3)	0.2539 (6)	0.8227 (3)	0.0379 (14)
H11	0.1364	0.3153	0.8475	0.045*
C12	0.1315 (3)	0.2653 (5)	0.7627 (3)	0.0334 (13)
H12	0.1041	0.3370	0.7461	0.040*
C13	0.1030 (3)	−0.0805 (5)	0.6262 (3)	0.0394 (14)
H13A	0.0839	−0.0730	0.5829	0.047*
H13B	0.1215	−0.1676	0.6343	0.047*
C14	0.0411 (4)	−0.0619 (6)	0.6559 (3)	0.0504 (18)
H14A	0.0601	−0.0263	0.6959	0.061*
H14B	0.0189	−0.1448	0.6607	0.061*
C15	−0.0177 (4)	0.0262 (6)	0.6211 (4)	0.058 (2)
H15A	−0.0363	−0.0070	0.5806	0.070*
H15B	−0.0589	0.0319	0.6410	0.070*
C16	0.0700 (3)	0.4605 (5)	0.6291 (2)	0.0291 (12)
C17	0.0256 (3)	0.5744 (5)	0.6235 (3)	0.0404 (14)
H17A	0.0255	0.6155	0.5856	0.061*
H17B	0.0459	0.6322	0.6561	0.061*

H17C	−0.0244	0.5521	0.6252	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0314 (4)	0.0225 (3)	0.0273 (4)	0.0038 (3)	0.0086 (3)	0.0016 (3)
Cl1	0.0357 (8)	0.0375 (7)	0.0332 (7)	−0.0068 (6)	0.0120 (6)	−0.0047 (6)
Cl2	0.0440 (9)	0.0379 (8)	0.0365 (8)	0.0053 (6)	0.0074 (7)	0.0025 (6)
N1	0.030 (2)	0.020 (2)	0.030 (2)	0.0003 (18)	0.0085 (19)	−0.0011 (18)
N2	0.022 (2)	0.032 (2)	0.030 (2)	−0.0014 (19)	0.0068 (19)	−0.002 (2)
N3	0.036 (2)	0.027 (2)	0.017 (2)	0.0041 (19)	0.0062 (18)	0.0031 (18)
N4	0.041 (3)	0.032 (3)	0.033 (3)	0.008 (2)	0.009 (2)	−0.001 (2)
O1	0.021 (2)	0.044 (3)	0.068 (3)	0.004 (2)	−0.003 (2)	0.011 (2)
O2	0.053 (3)	0.069 (3)	0.082 (4)	−0.030 (3)	0.007 (3)	0.012 (3)
O3	0.031 (2)	0.045 (2)	0.051 (3)	−0.0031 (19)	0.0049 (19)	0.009 (2)
O4	0.044 (3)	0.055 (3)	0.074 (3)	0.006 (2)	0.018 (2)	−0.026 (3)
O5	0.072 (3)	0.077 (3)	0.021 (2)	0.001 (3)	0.010 (2)	0.000 (2)
O6	0.072 (4)	0.147 (6)	0.034 (3)	0.040 (4)	0.005 (3)	0.016 (3)
O7	0.128 (6)	0.089 (4)	0.060 (4)	0.026 (4)	0.025 (4)	−0.015 (3)
O8	0.53 (2)	0.092 (6)	0.131 (9)	−0.135 (10)	0.107 (12)	−0.010 (6)
O9	0.078 (5)	0.55 (2)	0.059 (5)	0.122 (9)	0.014 (4)	0.020 (8)
C1	0.038 (3)	0.031 (3)	0.029 (3)	0.003 (2)	0.007 (2)	0.005 (2)
C2	0.041 (3)	0.042 (3)	0.027 (3)	−0.002 (3)	0.006 (3)	0.003 (3)
C3	0.041 (3)	0.039 (3)	0.029 (3)	0.000 (3)	0.011 (3)	0.000 (3)
C4	0.033 (3)	0.036 (3)	0.033 (3)	0.004 (2)	0.007 (2)	−0.003 (3)
C5	0.022 (3)	0.024 (2)	0.027 (3)	−0.006 (2)	0.000 (2)	0.001 (2)
C6	0.031 (3)	0.030 (3)	0.033 (3)	0.007 (2)	0.007 (2)	0.001 (2)
C7	0.029 (3)	0.029 (3)	0.032 (3)	0.005 (2)	0.007 (2)	0.004 (2)
C8	0.024 (3)	0.033 (3)	0.029 (3)	−0.006 (2)	0.008 (2)	0.002 (2)
C9	0.039 (3)	0.038 (3)	0.035 (3)	0.001 (3)	0.009 (3)	0.005 (3)
C10	0.053 (4)	0.044 (3)	0.024 (3)	−0.011 (3)	0.009 (3)	0.003 (3)
C11	0.044 (4)	0.036 (3)	0.036 (3)	−0.008 (3)	0.013 (3)	0.000 (3)
C12	0.042 (3)	0.031 (3)	0.031 (3)	0.002 (3)	0.016 (3)	0.002 (2)
C13	0.034 (3)	0.028 (3)	0.055 (4)	−0.002 (2)	0.006 (3)	0.007 (3)
C14	0.044 (4)	0.034 (3)	0.077 (5)	−0.007 (3)	0.023 (4)	0.010 (3)
C15	0.032 (4)	0.043 (4)	0.099 (6)	−0.002 (3)	0.013 (4)	0.004 (4)
C16	0.034 (3)	0.030 (3)	0.023 (3)	0.002 (2)	0.007 (2)	0.001 (2)
C17	0.036 (3)	0.032 (3)	0.052 (4)	0.010 (3)	0.010 (3)	−0.001 (3)

Geometric parameters (Å, º)

Cu1—N1	1.986 (4)	C3—H3	0.9500
Cu1—N3	1.991 (4)	C4—C5	1.386 (7)
Cu1—N4	1.997 (5)	C4—H4	0.9500
Cu1—N2	2.021 (4)	C5—C6	1.500 (7)
Cu1—O1	2.232 (4)	C6—H6A	0.9900
Cu1—O3	2.868 (4)	C6—H6B	0.9900
Cl1—O5	1.413 (4)	C7—C8	1.505 (7)

Cl1—O2	1.420 (5)	C7—H7A	0.9900
Cl1—O4	1.421 (4)	C7—H7B	0.9900
Cl1—O3	1.436 (4)	C8—C9	1.387 (8)
Cl2—O8	1.330 (8)	C9—C10	1.385 (8)
Cl2—O9	1.330 (7)	C9—H9	0.9500
Cl2—O6	1.389 (5)	C10—C11	1.368 (8)
Cl2—O7	1.405 (5)	C10—H10	0.9500
N1—C1	1.333 (7)	C11—C12	1.363 (8)
N1—C5	1.349 (6)	C11—H11	0.9500
N2—C7	1.493 (7)	C12—H12	0.9500
N2—C6	1.495 (7)	C13—C14	1.496 (8)
N2—C13	1.501 (7)	C13—H13A	0.9900
N3—C12	1.328 (7)	C13—H13B	0.9900
N3—C8	1.346 (7)	C14—C15	1.532 (9)
N4—C16	1.126 (7)	C14—H14A	0.9900
O1—C15	1.434 (8)	C14—H14B	0.9900
O1—H1A	0.73 (6)	C15—H15A	0.9900
C1—C2	1.377 (8)	C15—H15B	0.9900
C1—H1	0.9500	C16—C17	1.459 (7)
C2—C3	1.381 (8)	C17—H17A	0.9800
C2—H2	0.9500	C17—H17B	0.9800
C3—C4	1.374 (8)	C17—H17C	0.9800

N1—Cu1—N3	161.51 (18)	N2—C6—C5	109.8 (4)
N1—Cu1—N4	95.48 (18)	N2—C6—H6A	109.7
N3—Cu1—N4	95.08 (18)	C5—C6—H6A	109.7
N1—Cu1—N2	84.12 (17)	N2—C6—H6B	109.7
N3—Cu1—N2	84.88 (17)	C5—C6—H6B	109.7
N4—Cu1—N2	178.30 (19)	H6A—C6—H6B	108.2
N1—Cu1—O1	99.08 (19)	N2—C7—C8	112.0 (4)
N3—Cu1—O1	96.80 (19)	N2—C7—H7A	109.2
N4—Cu1—O1	85.79 (19)	C8—C7—H7A	109.2
N2—Cu1—O1	95.91 (17)	N2—C7—H7B	109.2
O5—Cl1—O2	111.0 (3)	C8—C7—H7B	109.2
O5—Cl1—O4	109.3 (3)	H7A—C7—H7B	107.9
O2—Cl1—O4	110.3 (3)	N3—C8—C9	120.6 (5)
O5—Cl1—O3	108.4 (3)	N3—C8—C7	117.5 (5)
O2—Cl1—O3	108.6 (3)	C9—C8—C7	121.8 (5)
O4—Cl1—O3	109.2 (3)	C10—C9—C8	118.8 (6)
O8—Cl2—O9	106.9 (9)	C10—C9—H9	120.6
O8—Cl2—O6	110.8 (6)	C8—C9—H9	120.6
O9—Cl2—O6	109.5 (4)	C11—C10—C9	119.4 (6)
O8—Cl2—O7	104.8 (6)	C11—C10—H10	120.3
O9—Cl2—O7	111.0 (6)	C9—C10—H10	120.3
O6—Cl2—O7	113.5 (4)	C12—C11—C10	119.1 (6)
C1—N1—C5	119.6 (5)	C12—C11—H11	120.5
C1—N1—Cu1	127.6 (4)	C10—C11—H11	120.5
C5—N1—Cu1	112.8 (3)	N3—C12—C11	122.4 (5)

C7—N2—C6	111.8 (4)	N3—C12—H12	118.8
C7—N2—C13	111.0 (4)	C11—C12—H12	118.8
C6—N2—C13	107.5 (4)	C14—C13—N2	116.2 (5)
C7—N2—Cu1	108.0 (3)	C14—C13—H13A	108.2
C6—N2—Cu1	106.7 (3)	N2—C13—H13A	108.2
C13—N2—Cu1	111.8 (3)	C14—C13—H13B	108.2
C12—N3—C8	119.7 (5)	N2—C13—H13B	108.2
C12—N3—Cu1	127.3 (4)	H13A—C13—H13B	107.4
C8—N3—Cu1	112.9 (3)	C13—C14—C15	112.6 (6)
C16—N4—Cu1	162.4 (5)	C13—C14—H14A	109.1
C15—O1—Cu1	125.4 (4)	C15—C14—H14A	109.1
C15—O1—H1A	98 (4)	C13—C14—H14B	109.1
Cu1—O1—H1A	130 (5)	C15—C14—H14B	109.1
N1—C1—C2	122.0 (5)	H14A—C14—H14B	107.8
N1—C1—H1	119.0	O1—C15—C14	108.4 (5)
C2—C1—H1	119.0	O1—C15—H15A	110.0
C1—C2—C3	118.5 (5)	C14—C15—H15A	110.0
C1—C2—H2	120.8	O1—C15—H15B	110.0
C3—C2—H2	120.8	C14—C15—H15B	110.0
C4—C3—C2	120.0 (5)	H15A—C15—H15B	108.4
C4—C3—H3	120.0	N4—C16—C17	179.1 (6)
C2—C3—H3	120.0	C16—C17—H17A	109.5
C3—C4—C5	118.7 (5)	C16—C17—H17B	109.5
C3—C4—H4	120.7	H17A—C17—H17B	109.5
C5—C4—H4	120.7	C16—C17—H17C	109.5
N1—C5—C4	121.1 (5)	H17A—C17—H17C	109.5
N1—C5—C6	116.8 (5)	H17B—C17—H17C	109.5
C4—C5—C6	122.0 (5)		

N3—Cu1—N1—C1	−137.9 (6)	N4—Cu1—O1—C15	−170.7 (6)
N4—Cu1—N1—C1	−13.4 (5)	N2—Cu1—O1—C15	9.4 (6)
N2—Cu1—N1—C1	168.3 (5)	Cu1—N1—C1—C2	179.7 (4)
O1—Cu1—N1—C1	73.2 (5)	Cu1—N1—C5—C4	179.2 (4)
N3—Cu1—N1—C5	41.3 (7)	C1—N1—C5—C6	175.0 (5)
N4—Cu1—N1—C5	165.9 (4)	Cu1—N1—C5—C6	−4.3 (6)
N2—Cu1—N1—C5	−12.5 (3)	C3—C4—C5—C6	−174.2 (5)
O1—Cu1—N1—C5	−107.5 (3)	C7—N2—C6—C5	−151.1 (4)
N1—Cu1—N2—C7	145.7 (3)	C13—N2—C6—C5	86.9 (5)
N3—Cu1—N2—C7	−19.4 (3)	Cu1—N2—C6—C5	−33.2 (5)
O1—Cu1—N2—C7	−115.7 (3)	N1—C5—C6—N2	25.8 (6)
N1—Cu1—N2—C6	25.3 (3)	C4—C5—C6—N2	−157.7 (5)
N3—Cu1—N2—C6	−139.8 (3)	C6—N2—C7—C8	139.1 (4)
O1—Cu1—N2—C6	123.9 (3)	C13—N2—C7—C8	−100.9 (5)
N1—Cu1—N2—C13	−91.9 (4)	Cu1—N2—C7—C8	21.9 (5)
N3—Cu1—N2—C13	103.0 (4)	C12—N3—C8—C9	−2.4 (8)
O1—Cu1—N2—C13	6.6 (4)	Cu1—N3—C8—C9	172.8 (4)
N1—Cu1—N3—C12	134.6 (6)	C12—N3—C8—C7	−179.2 (5)
N4—Cu1—N3—C12	10.0 (5)	N2—C7—C8—N3	−12.6 (7)

N2—Cu1—N3—C12	−171.7 (5)	N2—C7—C8—C9	170.7 (5)
O1—Cu1—N3—C12	−76.3 (5)	C7—C8—C9—C10	178.1 (5)
N1—Cu1—N3—C8	−40.2 (7)	C9—C10—C11—C12	−2.7 (9)
N4—Cu1—N3—C8	−164.8 (4)	Cu1—N3—C12—C11	−173.7 (4)
N2—Cu1—N3—C8	13.5 (4)	C7—N2—C13—C14	69.5 (6)
O1—Cu1—N3—C8	108.9 (4)	C6—N2—C13—C14	−168.0 (5)
N1—Cu1—N4—C16	102.7 (16)	Cu1—N2—C13—C14	−51.2 (6)
N3—Cu1—N4—C16	−92.5 (16)	N2—C13—C14—C15	91.7 (7)
N1—Cu1—O1—C15	94.4 (6)	Cu1—O1—C15—C14	15.4 (9)
N3—Cu1—O1—C15	−76.1 (6)	C13—C14—C15—O1	−63.0 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O9	0.74 (5)	2.46 (5)	3.090 (12)	145 (5)