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Crystal structure of *trans*-aqua(perchlorato-κO)-bis(propane-1,3-diamine-κ^2N,N')copper(II) perchlorate

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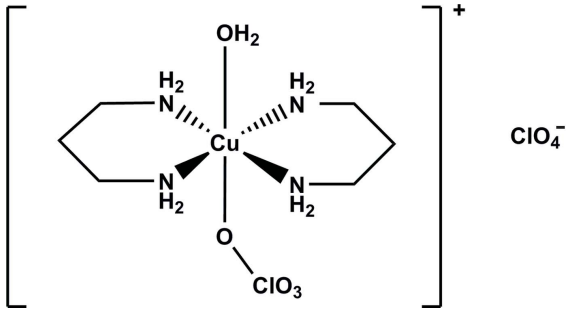
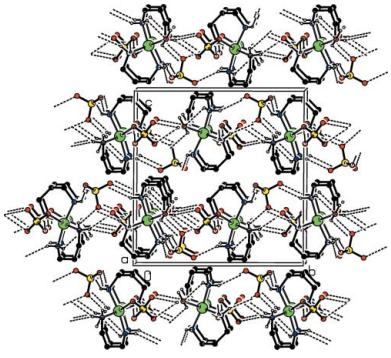
In the title compound, $[Cu(ClO_4)(C_3H_{10}N_2)_2(H_2O)]ClO_4$, the Cu^{II} atom has a distorted octahedral coordination sphere and is coordinated by the N atoms of two propane-1,3-diamine ligands in the equatorial plane. The axial positions are occupied by a water O atom and an O atom of a disordered perchlorate anion [occupancy ratio 0.631 (9):0.369 (9)]. In the crystal, the various components are linked *via* O—H···O, N—H···O and C—H···O hydrogen bonds, forming sheets lying parallel to (001).

1. Chemical context

There have been numerous reports of bis(propane-1,3-diamine)copper(II) complexes, essentially with the copper atom coordinated by the N atoms of the ligands in the equatorial plane of the copper octahedral coordination sphere and with two identical O-containing ligands in the axial positions, for example, *trans*-diaquabis(propane-1,3-diamine-κ^2N,N')copper(II) dithionate (Kim *et al.*, 2003) and bis[aqua(1,3-diaminopropane-κ^2N,N')]copper(II) difluoride (Emsley *et al.*, 1988). In order to further develop the coordination chemistry of such copper complexes, we report herein on the synthesis and crystal structure of the title complex, which has two different ligands in the axial positions of the octahedral coordination sphere of the copper atom.





2. Structural commentary

The molecular structure of the title complex is illustrated in Fig. 1. The Cu^{II} atom has a distorted octahedral coordination sphere, reflecting the characteristic Jahn–Teller distortion. It is coordinated by the N atoms of two propane-1,3-diamine ligands in the equatorial plane with Cu—N bond lengths varying between 2.003 (4)–2.023 (3) Å. The axial positions are

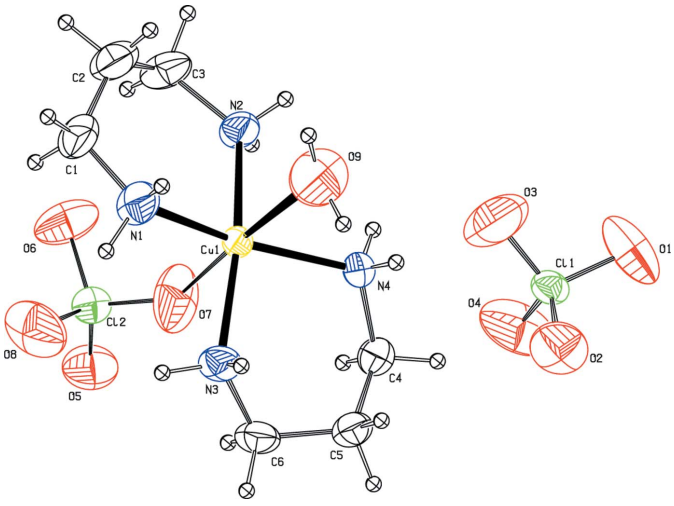


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The minor components of the disordered coordinating perchlorate anion have been omitted for clarity.

occupied by the water O9 atom and by atom O7 of a disordered perchlorate anion [occupancy ratio 0.631 (9):0.369 (9)], with Cu—O bond lengths of 2.585 (6) and 2.680 (10) Å, respectively.

3. Supramolecular features

In the crystal, the various components are linked *via* O—H···O, N—H···O and C—H···O hydrogen bonds forming sheets lying parallel to (001); see Table 1 and Fig. 2.

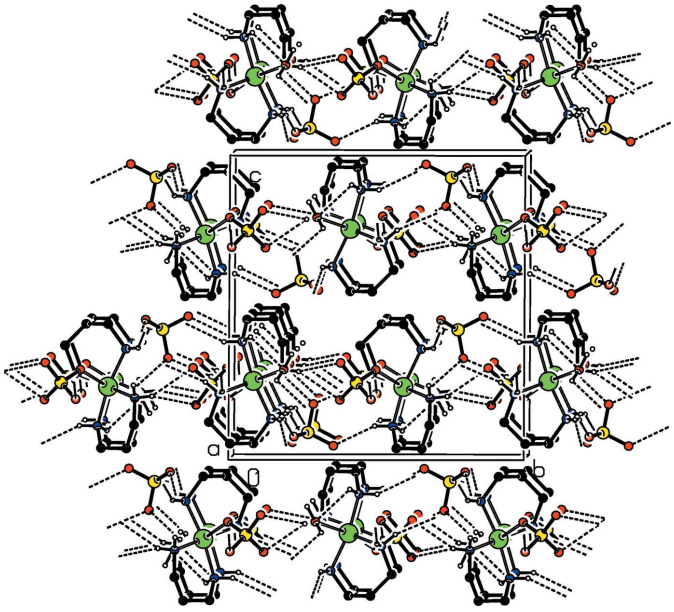


Figure 2
A view along the *a* axis of the crystal structure of the title compound. O—H···O and N—H···O hydrogen bonds are shown as dashed lines (see Table 1 for details; the minor components of the disordered coordinating perchlorate anion and the C-bound H atoms have been omitted for clarity)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H9*B*···O3^{i}	0.90 (2)	2.38 (11)	2.917 (9)	118 (9)
N1—H1*C*···O1	0.90	2.22	3.040 (7)	151
N1—H1*D*···O1^{ii}	0.90	2.69	3.511 (8)	151
N1—H1*D*···O9	0.90	2.41	2.927 (8)	117
N2—H2*C*···O5^{iii}	0.90	2.58	3.443 (12)	162
N2—H2*C*···O8^{iii}	0.90	2.42	3.183 (10)	143
N2—H2*C*···O5′^{iii}	0.90	2.39	3.23 (3)	156
N2—H2*D*···O3^{iii}	0.90	2.70	3.449 (11)	141
N3—H3*C*···O6^{iv}	0.90	2.15	3.014 (9)	160
N3—H3*C*···O7′^{iv}	0.90	2.36	3.246 (17)	169
N3—H3*D*···O3	0.90	2.28	3.137 (8)	160
N4—H4*C*···O2^{iii}	0.90	2.35	3.127 (6)	144
N4—H4*D*···O4^{i}	0.90	2.45	3.223 (7)	145
C4—H4*A*···O5′^{v}	0.97	2.47	3.264 (14)	139
C5—H5*B*···O4^{i}	0.97	2.63	3.368 (7)	133

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

4. Synthesis and crystallization

The complex was prepared by mixing copper(II) perchlorate hexahydrate with 1,3-diaminopropane in a (1:2) molar ratio. $Cu(ClO_4)_2{\cdot}6H_2O$ (3.7 g, 1 *M*) was dissolved in 15 ml of warm water. After an hour, about 10 ml of an ethanol solution of 1,3-diaminopropane (1.48 g, 2*M*) was added dropwise with continuous stirring. This solution was then filtered to remove

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu(ClO_4)(C_3H_{10}N_2)_2(H_2O)]ClO_4$
M_r	428.72
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	7.8563 (4), 14.2936 (6), 14.8769 (7)
β (°)	100.022 (5)
V (Å^3)	1645.11 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.70
Crystal size (mm)	0.30 × 0.30 × 0.25
Data collection	
Diffractometer	Oxford Diffraction Xcalibur with an Eos detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min}, T_{max}	0.607, 0.654
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7573, 2900, 2353
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.046, 0.127, 1.06
No. of reflections	2900
No. of parameters	242
No. of restraints	109
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.60, −0.42

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2009), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

any impurities and the solution was kept over P_2O_5 in a desiccator. Finally, violet–purple-coloured crystals suitable for X-ray diffraction analysis were harvested and washed repeatedly with cold water (yield 70%).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The water H atoms were located in a difference Fourier map and refined with a distance restraint, O—H = 0.90 (2) Å, and with U_{iso}(H) = 1.5U_{eq}(O). The N -and C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H = 0.90 and C—H = 0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(N,C). The disordered coordinating perchlorate anion, involving atom Cl2, was refined with an occupancy ratio of 0.631 (9):0.369 (9).

Acknowledgements

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supporting information

Acta Cryst. (2014). E**70**, 438-440 [doi:10.1107/S1600536814023496]

Crystal structure of *trans*-aqua(perchlorato-κO)bis(propane-1,3-diamine-$\kappa^2 N,N'$)copper(II) perchlorate

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Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

trans-Aqua(perchlorato-κO)bis(propane-1,3-diamine-$\kappa^2 N,N'$)copper(II) perchlorate

Crystal data

$[Cu(ClO_4)(C_3H_{10}N_2)_2(H_2O)]ClO_4$
$M_r = 428.72$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.8563$ (4) Å
$b = 14.2936$ (6) Å
$c = 14.8769$ (7) Å
$\beta = 100.022$ (5)°
$V = 1645.11$ (13) Å^3
$Z = 4$
$F(000) = 884$
$D_x = 1.731$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2353 reflections
$\theta = 3.8$–$25.0°$
$\mu = 1.70$ mm^{-1}
$T = 293$ K
Block, violet-purple
0.30 × 0.30 × 0.25 mm

Data collection

Oxford diffraction Xcalibur diffractometer with an Eos detector
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min} = 0.607$, $T_{max} = 0.654$
7573 measured reflections
2900 independent reflections
2353 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.8°$
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.127$
$S = 1.06$
2900 reflections
242 parameters
109 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

$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 1.2858P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.2060 (10)	0.0648 (5)	0.4655 (4)	0.0879 (19)	
H1A	0.2841	0.0599	0.5234	0.105*	
H1B	0.1231	0.0142	0.4630	0.105*	
C2	0.1130 (10)	0.1523 (5)	0.4648 (4)	0.099 (2)	
H2A	0.0517	0.1508	0.5160	0.119*	
H2B	0.1985	0.2017	0.4771	0.119*	
C3	−0.0098 (8)	0.1800 (5)	0.3854 (4)	0.0846 (17)	
H3A	−0.0506	0.2423	0.3965	0.101*	
H3B	−0.1084	0.1383	0.3802	0.101*	
C4	0.1631 (8)	0.0875 (3)	0.0573 (3)	0.0667 (14)	
H4A	0.1641	0.1259	0.0037	0.080*	
H4B	0.0489	0.0602	0.0524	0.080*	
C5	0.2934 (7)	0.0105 (3)	0.0589 (3)	0.0659 (13)	
H5A	0.2758	−0.0197	−0.0004	0.079*	
H5B	0.4083	0.0376	0.0693	0.079*	
C6	0.2841 (8)	−0.0610 (3)	0.1296 (3)	0.0700 (14)	
H6A	0.1671	−0.0851	0.1218	0.084*	
H6B	0.3597	−0.1126	0.1208	0.084*	
N1	0.3041 (7)	0.0504 (4)	0.3943 (3)	0.0860 (15)	
H1C	0.3285	−0.0111	0.3940	0.103*	
H1D	0.4054	0.0803	0.4113	0.103*	
N2	0.0484 (6)	0.1812 (3)	0.2978 (3)	0.0705 (12)	
H2C	0.0951	0.2380	0.2925	0.085*	
H2D	−0.0471	0.1780	0.2546	0.085*	
N3	0.3333 (6)	−0.0259 (3)	0.2235 (3)	0.0678 (11)	
H3C	0.4473	−0.0136	0.2325	0.081*	
H3D	0.3180	−0.0730	0.2614	0.081*	
N4	0.1967 (6)	0.1474 (2)	0.1393 (2)	0.0573 (10)	
H4C	0.1117	0.1902	0.1342	0.069*	
H4D	0.2958	0.1786	0.1382	0.069*	
O1	0.3452 (8)	−0.1512 (3)	0.4593 (5)	0.149 (2)	
O2	0.1810 (6)	−0.2818 (4)	0.4266 (4)	0.1161 (16)	

O3	0.3230 (12)	−0.2194 (6)	0.3219 (5)	0.185 (3)	
O4	0.4749 (7)	−0.2926 (4)	0.4506 (5)	0.156 (3)	
Cl1	0.33528 (15)	−0.23745 (7)	0.41570 (8)	0.0557 (3)	
Cl2	−0.18163 (15)	−0.06425 (9)	0.24310 (7)	0.0576 (3)	
Cu1	0.21563 (6)	0.08711 (3)	0.26368 (3)	0.0411 (2)	
O5	−0.2890 (12)	−0.1162 (7)	0.1754 (6)	0.102 (3)	0.631 (9)
O6	−0.2845 (9)	−0.0126 (8)	0.2958 (6)	0.109 (3)	0.631 (9)
O7	−0.0828 (12)	−0.0013 (7)	0.2023 (6)	0.133 (4)	0.631 (9)
O8	−0.0665 (16)	−0.1226 (7)	0.3013 (6)	0.142 (4)	0.631 (9)
O5′	−0.188 (3)	−0.1082 (17)	0.1585 (9)	0.156 (9)	0.369 (9)
O6′	−0.0084 (12)	−0.0497 (11)	0.2830 (12)	0.117 (5)	0.369 (9)
O7′	−0.2628 (19)	0.0227 (8)	0.2243 (14)	0.131 (6)	0.369 (9)
O8′	−0.258 (2)	−0.1212 (13)	0.2983 (10)	0.138 (6)	0.369 (9)
O9	0.4814 (7)	0.1951 (5)	0.3062 (4)	0.133 (2)	
H9B	0.557 (10)	0.173 (8)	0.272 (6)	0.200*	
H9A	0.536 (11)	0.222 (7)	0.357 (4)	0.200*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.121 (5)	0.097 (4)	0.048 (3)	0.019 (4)	0.022 (3)	0.011 (3)
C2	0.141 (6)	0.105 (5)	0.058 (3)	0.035 (5)	0.032 (4)	−0.006 (3)
C3	0.081 (4)	0.101 (4)	0.076 (4)	0.024 (3)	0.026 (3)	−0.019 (3)
C4	0.092 (4)	0.062 (3)	0.045 (2)	0.005 (3)	0.009 (3)	0.003 (2)
C5	0.073 (3)	0.067 (3)	0.064 (3)	−0.004 (3)	0.028 (3)	−0.013 (2)
C6	0.081 (4)	0.054 (3)	0.076 (3)	0.015 (3)	0.017 (3)	−0.014 (2)
N1	0.115 (4)	0.086 (3)	0.056 (2)	0.043 (3)	0.013 (3)	0.019 (2)
N2	0.088 (3)	0.066 (3)	0.063 (2)	0.036 (2)	0.028 (2)	0.0098 (19)
N3	0.078 (3)	0.060 (2)	0.064 (2)	0.031 (2)	0.010 (2)	0.0014 (19)
N4	0.080 (3)	0.045 (2)	0.049 (2)	0.0049 (19)	0.0173 (19)	0.0063 (15)
O1	0.138 (5)	0.072 (3)	0.221 (6)	0.001 (3)	−0.014 (4)	−0.046 (4)
O2	0.078 (3)	0.114 (3)	0.163 (5)	−0.024 (3)	0.039 (3)	0.001 (3)
O3	0.245 (9)	0.197 (7)	0.139 (5)	0.046 (6)	0.107 (6)	0.062 (5)
O4	0.080 (3)	0.107 (4)	0.276 (8)	0.042 (3)	0.021 (4)	0.059 (5)
Cl1	0.0524 (6)	0.0451 (6)	0.0733 (7)	0.0054 (5)	0.0212 (6)	0.0074 (5)
Cl2	0.0526 (6)	0.0603 (7)	0.0599 (7)	−0.0013 (5)	0.0092 (5)	−0.0059 (5)
Cu1	0.0435 (3)	0.0393 (3)	0.0415 (3)	0.0075 (2)	0.0096 (2)	0.00435 (19)
O5	0.104 (6)	0.099 (5)	0.097 (6)	−0.017 (5)	0.002 (5)	−0.030 (5)
O6	0.069 (4)	0.162 (9)	0.098 (5)	0.007 (5)	0.019 (4)	−0.049 (6)
O7	0.109 (7)	0.167 (8)	0.127 (7)	−0.064 (6)	0.037 (6)	0.023 (6)
O8	0.185 (10)	0.101 (6)	0.117 (6)	0.043 (7)	−0.040 (7)	0.016 (5)
O5′	0.23 (2)	0.172 (15)	0.059 (8)	0.010 (18)	0.020 (12)	−0.023 (9)
O6′	0.045 (6)	0.115 (11)	0.184 (14)	−0.002 (7)	−0.002 (7)	0.008 (10)
O7′	0.108 (11)	0.064 (7)	0.203 (16)	0.002 (7)	−0.022 (12)	−0.012 (9)
O8′	0.128 (12)	0.182 (15)	0.109 (10)	−0.019 (12)	0.036 (9)	0.044 (10)
O9	0.118 (4)	0.150 (5)	0.133 (5)	−0.054 (4)	0.024 (4)	−0.030 (4)

Geometric parameters (Å, º)

C1—N1	1.429 (7)	N2—H2C	0.9000
C1—C2	1.447 (8)	N2—H2D	0.9000
C1—H1A	0.9700	N3—Cu1	2.003 (4)
C1—H1B	0.9700	N3—H3C	0.9000
C2—C3	1.445 (9)	N3—H3D	0.9000
C2—H2A	0.9700	N4—Cu1	2.023 (3)
C2—H2B	0.9700	N4—H4C	0.9000
C3—N2	1.454 (6)	N4—H4D	0.9000
C3—H3A	0.9700	O1—Cl1	1.388 (5)
C3—H3B	0.9700	O2—Cl1	1.402 (4)
C4—N4	1.476 (6)	O3—Cl1	1.406 (6)
C4—C5	1.500 (7)	O4—Cl1	1.377 (5)
C4—H4A	0.9700	Cl2—O8′	1.368 (11)
C4—H4B	0.9700	Cl2—O7	1.395 (7)
C5—C6	1.478 (7)	Cl2—O5′	1.399 (12)
C5—H5A	0.9700	Cl2—O6′	1.402 (9)
C5—H5B	0.9700	Cl2—O7′	1.403 (10)
C6—N3	1.471 (6)	Cl2—O5	1.408 (7)
C6—H6A	0.9700	Cl2—O8	1.411 (7)
C6—H6B	0.9700	Cl2—O6	1.425 (6)
N1—Cu1	2.015 (4)	O9—H9B	0.90 (2)
N1—H1C	0.9000	O9—H9A	0.89 (2)
N1—H1D	0.9000	Cu1—09	2.585 (6)
N2—Cu1	2.006 (4)	Cu1—O7	2.680 (1)
N1—C1—C2	117.2 (5)	C6—N3—H3D	107.3
N1—C1—H1A	108.0	Cu1—N3—H3D	107.3
C2—C1—H1A	108.0	H3C—N3—H3D	106.9
N1—C1—H1B	108.0	C4—N4—Cu1	118.9 (3)
C2—C1—H1B	108.0	C4—N4—H4C	107.6
H1A—C1—H1B	107.3	Cu1—N4—H4C	107.6
C3—C2—C1	120.5 (5)	C4—N4—H4D	107.6
C3—C2—H2A	107.2	Cu1—N4—H4D	107.6
C1—C2—H2A	107.2	H4C—N4—H4D	107.0
C3—C2—H2B	107.2	O4—Cl1—O1	110.8 (4)
C1—C2—H2B	107.2	O4—Cl1—O2	110.2 (3)
H2A—C2—H2B	106.8	O1—Cl1—O2	109.1 (4)
C2—C3—N2	117.8 (5)	O4—Cl1—O3	113.1 (5)
C2—C3—H3A	107.9	O1—Cl1—O3	106.8 (5)
N2—C3—H3A	107.9	O2—Cl1—O3	106.6 (5)
C2—C3—H3B	107.9	O8′—Cl2—O7	169.0 (9)
N2—C3—H3B	107.9	O8′—Cl2—O5′	108.7 (11)
H3A—C3—H3B	107.2	O7—Cl2—O5′	80.5 (10)
N4—C4—C5	112.9 (4)	O8′—Cl2—O6′	109.2 (10)
N4—C4—H4A	109.0	O7—Cl2—O6′	61.0 (7)
C5—C4—H4A	109.0	O5′—Cl2—O6′	109.2 (10)

N4—C4—H4B	109.0	O8′—Cl2—O7′	114.5 (10)
C5—C4—H4B	109.0	O7—Cl2—O7′	67.0 (8)
H4A—C4—H4B	107.8	O5′—Cl2—O7′	105.9 (13)
C6—C5—C4	113.7 (4)	O6′—Cl2—O7′	109.1 (8)
C6—C5—H5A	108.8	O8′—Cl2—O5	81.0 (9)
C4—C5—H5A	108.8	O7—Cl2—O5	109.8 (6)
C6—C5—H5B	108.8	O5′—Cl2—O5	36.4 (9)
C4—C5—H5B	108.8	O6′—Cl2—O5	142.9 (7)
H5A—C5—H5B	107.7	O7′—Cl2—O5	97.5 (8)
N3—C6—C5	113.7 (4)	O8′—Cl2—O8	65.3 (8)
N3—C6—H6A	108.8	O7—Cl2—O8	107.6 (6)
C5—C6—H6A	108.8	O5′—Cl2—O8	101.9 (11)
N3—C6—H6B	108.8	O6′—Cl2—O8	50.0 (7)
C5—C6—H6B	108.8	O7′—Cl2—O8	150.1 (8)
H6A—C6—H6B	107.7	O5—Cl2—O8	111.6 (6)
C1—N1—Cu1	122.5 (4)	O8′—Cl2—O6	68.1 (8)
C1—N1—H1C	106.7	O7—Cl2—O6	108.5 (6)
Cu1—N1—H1C	106.7	O5′—Cl2—O6	142.2 (11)
C1—N1—H1D	106.7	O6′—Cl2—O6	106.9 (7)
Cu1—N1—H1D	106.7	O7′—Cl2—O6	50.9 (8)
H1C—N1—H1D	106.6	O5—Cl2—O6	109.9 (5)
C3—N2—Cu1	122.8 (3)	O8—Cl2—O6	109.5 (6)
C3—N2—H2C	106.6	N3—Cu1—N2	166.5 (2)
Cu1—N2—H2C	106.6	N3—Cu1—N1	88.76 (17)
C3—N2—H2D	106.6	N2—Cu1—N1	93.53 (17)
Cu1—N2—H2D	106.6	N3—Cu1—N4	91.99 (15)
H2C—N2—H2D	106.6	N2—Cu1—N4	89.94 (15)
C6—N3—Cu1	120.0 (3)	N1—Cu1—N4	161.9 (2)
C6—N3—H3C	107.3	H9B—O9—H9A	111 (3)
Cu1—N3—H3C	107.3		

N1—C1—C2—C3	56.0 (10)	C6—N3—Cu1—N4	−35.4 (4)
C1—C2—C3—N2	−53.1 (10)	C3—N2—Cu1—N3	79.8 (9)
N4—C4—C5—C6	67.7 (6)	C3—N2—Cu1—N1	−19.6 (5)
C4—C5—C6—N3	−66.7 (6)	C3—N2—Cu1—N4	178.1 (5)
C2—C1—N1—Cu1	−41.1 (9)	C1—N1—Cu1—N3	−144.4 (5)
C2—C3—N2—Cu1	35.8 (8)	C1—N1—Cu1—N2	22.4 (5)
C5—C6—N3—Cu1	54.2 (6)	C1—N1—Cu1—N4	123.0 (6)
C5—C4—N4—Cu1	−55.5 (5)	C4—N4—Cu1—N3	36.2 (4)
C6—N3—Cu1—N2	62.7 (8)	C4—N4—Cu1—N2	−130.4 (4)
C6—N3—Cu1—N1	162.7 (4)	C4—N4—Cu1—N1	128.3 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H9*B*···O3^{i}	0.90 (2)	2.38 (11)	2.917 (9)	118 (9)
N1—H1*C*···O1	0.90	2.22	3.040 (7)	151
N1—H1*D*···O1^{ii}	0.90	2.69	3.511 (8)	151

N1—H1*D*···O9	0.90	2.41	2.927 (8)	117
N2—H2*C*···O5^{iii}	0.90	2.58	3.443 (12)	162
N2—H2*C*···O8^{iii}	0.90	2.42	3.183 (10)	143
N2—H2*C*···O5′^{iii}	0.90	2.39	3.23 (3)	156
N2—H2*D*···O3^{iii}	0.90	2.70	3.449 (11)	141
N3—H3*C*···O6^{iv}	0.90	2.15	3.014 (9)	160
N3—H3*C*···O7′^{iv}	0.90	2.36	3.246 (17)	169
N3—H3*D*···O3	0.90	2.28	3.137 (8)	160
N4—H4*C*···O2^{iii}	0.90	2.35	3.127 (6)	144
N4—H4*D*···O4^{i}	0.90	2.45	3.223 (7)	145
C4—H4*A*···O5′^{v}	0.97	2.47	3.264 (14)	139
C5—H5*B*···O4^{i}	0.97	2.63	3.368 (7)	133

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