

Diaqua(2,2'-bipyridine- $\kappa^2 N,N'$)bis-(perchlorato- κO)copper(II)

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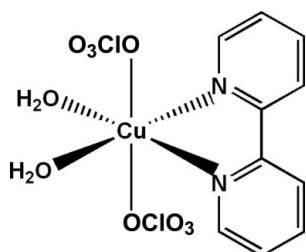
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.002$ Å; R factor = 0.030; wR factor = 0.080; data-to-parameter ratio = 21.6.

The central CuN_2O_4 motif of the title compound, $[Cu(ClO_4)_2(C_{10}H_8N_2)(H_2O)_2]$, exhibits a Jahn–Teller-distorted octahedral geometry around the metal atom, showing a considerably long Cu–O bond distance of 2.5058 (12) Å towards the second perchlorate group, giving a (4 + 1+1)-type coordination mode. In the crystal, the components are linked via intermolecular O–H···O hydrogen bonds, forming layers parallel to (001). Additional stabilization within these layers is provided by π – π [centroid–centroid distances of 3.7848 (9)–4.4231 (9) Å] stacking interactions.

Related literature

For applications of related compounds, see: Kurzak *et al.* (1999). For the coordination spheres of copper in related compounds, see: Hathaway (1973). For hydrogen-bond motifs, see: Bernstein *et al.* (1995); Etter *et al.* (1990).



Experimental

Crystal data

$[Cu(ClO_4)_2(C_{10}H_8N_2)(H_2O)_2]$ $M_r = 454.67$

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Monoclinic, $P2_1/n$
 $a = 7.1378$ (4) Å
 $b = 12.7853$ (7) Å
 $c = 16.8033$ (11) Å
 $\beta = 92.025$ (6) $^\circ$
 $V = 1532.49$ (16) Å 3

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.83$ mm $^{-1}$
 $T = 296$ K
 $0.13 \times 0.07 \times 0.05$ mm

Data collection

Oxford Diffraction Xcalibur
Sapphire2 diffractometer
Absorption correction: multi-scan
(*CrysAlis RED*; Oxford
Diffraction, 2008)
 $T_{\min} = 0.580$, $T_{\max} = 1.000$

16487 measured reflections
5135 independent reflections
4239 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.080$
 $S = 1.05$
5135 reflections
238 parameters

H atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{\max} = 0.42$ e Å $^{-3}$
 $\Delta\rho_{\min} = -0.63$ e Å $^{-3}$

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W–H1W···O10 ⁱ	0.72 (2)	2.04 (2)	2.7078 (17)	155 (3)
O1W–H2W···O3 ⁱⁱ	0.88 (2)	1.89 (2)	2.7665 (17)	177.3 (18)
O2W–H3W···O3 ⁱⁱⁱ	0.76 (2)	2.13 (2)	2.8802 (18)	169 (2)
O2W–H4W···O4	0.78 (2)	2.37 (2)	2.9518 (19)	133 (2)
O2W–H4W···O7 ^{iv}	0.78 (2)	2.26 (3)	2.8349 (18)	132 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis CCD*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2292).

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supplementary materials

Acta Cryst. (2011). E67, m611-m612 [doi:10.1107/S1600536811013808]

Diaqua(2,2'-bipyridine- κ^2N,N')bis(perchlorato- κO)copper(II)

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Comment

Copper(II) complexes containing O, N-donor atoms are very important owing to their significant catalytic activity in the preparative oxygenation of phenols and other substances, and their significant antibacterial and anticancer activity (Kurzak *et al.*, 1999).

The asymmetric unit of (I), and the atomic numbering used, is illustrated in Fig. 1. The Cu^{II} atom is located in a Jahn-Teller distorted octahedral coordination environment with two N atoms from one 2,2'-bipyridine ligand (N1, N2) ($d(\text{Cu}—\text{N}) = 1.9723$ (13)–1.9805 (12) Å) and two O atoms from two water molecular adopting a planar arrangement ($d(\text{Cu}—\text{O}) = 1.9621$ (12)–1.9719 (12) Å). The Cu(II) center is displaced out of the N₂O₂ plane by 0.028 (2) Å in the direction of one of perchlorate ligand with $d(\text{Cu}—\text{O}9) = 2.3287$ (12) Å. The O atom of the second perchlorate group occupies a sixth coordination site at a longer distance of 2.5058 (12) Å, completing the overall (4 + 1 + 1) type coordination. O9 is situated slightly off the axial direct of the square pyramid, nevertheless it is close enough to the Cu atom (Hathaway, 1973). The bipyridine rings of the 2,2'-bipyridine ligand are twisted relative to each other at 2.2 (8)°.

The crystal structure can be described as alternating layers of polyhedral (ClO₄ tetrahedrals and CuN₂O₄ octahedrals) perpendicular to *c* axis (Fig. 2).

The crystal packing in (I) is governed by classical hydrogen bond, *viz.* water molecules and perchlorate (Table 1, Fig. 3). All water H atoms are involved in these hydrogen bonds. In the crystal, the components of the structure are linked *via* intermolecular O—H···O hydrogen bonds to form a two-dimensional layers parallel to (001) plane (Fig. 3). Additional stabilization within these layers is provided by π – π [3.7848 (9) Å to 4.4231 (9) Å] stacking interactions. These interaction bonds link the molecules within the layers and also link the layers together and reinforcing the cohesion of the structure.

The combination of these hydrogen bonds generates an alternating centrosymmetric rings in two-dimensional network which can be described by the graph-set motif R₄²(12) and R₄⁴(16) (Bernstein *et al.* 1995; Etter *et al.*, 1990).

Experimental

The title compound was prepared by adding a methanol solution (10 ml) of copper (II) acetate monohydrate (0.1 mmol) to a methanol solution (10 ml) of 2,2'-bipyridine (0.1 mmol) and (1 ml) the perchloric acid. The mixture was stirred for about 2 h at 323 K and filtered. The filtrate was slowly evaporated at room temperature to yield blue crystals of (I) suitable for X-ray analysis.

supplementary materials

Refinement

H atoms of water molecule were located in difference Fourier maps and refined isotropically using restraints $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The remaining H atoms were localized on Fourier maps but introduced in calculated positions and treated as riding on their parent atoms (C_{aryl}) with $\text{C}_{\text{aryl}}-\text{H}_{\text{aryl}}=0.93\text{\AA}$ and $U_{\text{iso}}(\text{H}_{\text{aryl}})=1.2U_{\text{eq}}(\text{C}_{\text{aryl}})$.

Figures

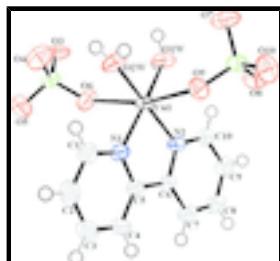


Fig. 1. (Farrugia, 1997) The asymmetric unit of the title compound with the atomic labeling scheme. Displacements are drawn at the 50% probability level.

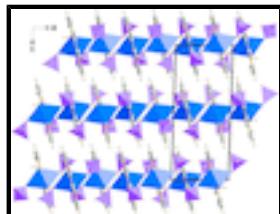


Fig. 2. (Brandenburg & Berndt, 2001) A diagram of the layered crystal packing in (I), viewed down the b axis, showing layers parallel to (001) with alternating polyhedrals (ClO_4 and CuN_2O_4).

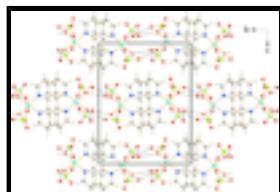


Fig. 3. (Brandenburg & Berndt, 2001) A part of crystal packing of (I) showing hydrogen bond connections in the same layer as dashed line.

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Crystal data

$[\text{Cu}(\text{ClO}_4)_2(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2]$	$F(000) = 916$
$M_r = 454.67$	$D_x = 1.971 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	$\text{Mo K}\alpha$ radiation, $\lambda = 0.7107 \text{ \AA}$
$a = 7.1378 (4) \text{ \AA}$	Cell parameters from 9763 reflections
$b = 12.7853 (7) \text{ \AA}$	$\theta = 3.0\text{--}32.3^\circ$
$c = 16.8033 (11) \text{ \AA}$	$\mu = 1.83 \text{ mm}^{-1}$
$\beta = 92.025 (6)^\circ$	$T = 296 \text{ K}$
$V = 1532.49 (16) \text{ \AA}^3$	Needle, blue
$Z = 4$	$0.13 \times 0.07 \times 0.05 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur Sapphire2 diffractometer	5135 independent reflections
Radiation source: Enhance (Mo) X-ray Source graphite	4239 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.034$
Detector resolution: 8.2632 pixels mm ⁻¹	$\theta_{\text{max}} = 32.3^\circ$, $\theta_{\text{min}} = 3.1^\circ$
ω scans	$h = -10 \rightarrow 6$
Absorption correction: multi-scan (<i>CrysAlis RED</i> ; Oxford Diffraction, 2008)	$k = -19 \rightarrow 19$
$T_{\text{min}} = 0.580$, $T_{\text{max}} = 1.000$	$l = -25 \rightarrow 25$
16487 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.030$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.080$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
5135 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
238 parameters	$\Delta\rho_{\text{max}} = 0.42 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.63 \text{ e \AA}^{-3}$

Special details

Experimental. CrysAlis RED, Oxford Diffraction Ltd. (Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm).

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.8677 (2)	0.16080 (13)	0.14228 (10)	0.0255 (3)
H1	0.8893	0.2282	0.1613	0.031*

supplementary materials

C2	0.8928 (3)	0.07755 (15)	0.19373 (11)	0.0302 (4)
H2	0.9318	0.0886	0.2465	0.036*
C3	0.8593 (3)	-0.02215 (14)	0.16589 (11)	0.0299 (4)
H3	0.8759	-0.0794	0.1995	0.036*
C4	0.8012 (2)	-0.03613 (13)	0.08784 (11)	0.0263 (3)
H4	0.7765	-0.1029	0.0681	0.032*
C5	0.7797 (2)	0.05028 (11)	0.03897 (10)	0.0189 (3)
C6	0.7203 (2)	0.04419 (11)	-0.04548 (9)	0.0181 (3)
C7	0.6861 (2)	-0.04880 (12)	-0.08553 (11)	0.0244 (3)
H7	0.6975	-0.1125	-0.059	0.029*
C8	0.6349 (2)	-0.04559 (13)	-0.16509 (11)	0.0283 (4)
H8	0.6092	-0.1071	-0.1929	0.034*
C9	0.6220 (2)	0.04947 (14)	-0.20331 (11)	0.0269 (3)
H9	0.589	0.0529	-0.2573	0.032*
C10	0.6588 (2)	0.13967 (12)	-0.16024 (10)	0.0226 (3)
H10	0.6518	0.2039	-0.1861	0.027*
N1	0.81339 (18)	0.14762 (10)	0.06591 (8)	0.0196 (2)
N2	0.70407 (17)	0.13722 (9)	-0.08243 (8)	0.0186 (2)
O1W	0.66836 (17)	0.36086 (9)	-0.09192 (8)	0.0237 (2)
H1W	0.568 (3)	0.3587 (18)	-0.0987 (14)	0.036*
H2W	0.691 (3)	0.4275 (19)	-0.0820 (14)	0.036*
O2W	0.86002 (18)	0.37137 (9)	0.05755 (9)	0.0274 (3)
H3W	0.958 (3)	0.394 (2)	0.0544 (15)	0.041*
H4W	0.805 (3)	0.415 (2)	0.0787 (15)	0.041*
O3	0.24885 (18)	0.43183 (9)	0.05923 (9)	0.0361 (3)
O4	0.51492 (18)	0.41771 (11)	0.14266 (8)	0.0363 (3)
O5	0.2632 (2)	0.30038 (12)	0.15559 (9)	0.0406 (3)
O6	0.45262 (17)	0.28891 (10)	0.04596 (8)	0.0313 (3)
O7	1.1044 (2)	0.43059 (10)	-0.13244 (9)	0.0389 (3)
O8	1.02596 (19)	0.27740 (10)	-0.20091 (8)	0.0322 (3)
O9	1.06594 (16)	0.27377 (10)	-0.06166 (7)	0.0256 (2)
O10	1.32354 (16)	0.29465 (11)	-0.14184 (8)	0.0324 (3)
Cu1	0.76523 (3)	0.258975 (14)	-0.013428 (12)	0.01792 (6)
Cl1	0.37148 (5)	0.35902 (3)	0.10177 (2)	0.02055 (8)
Cl2	1.12857 (5)	0.32027 (3)	-0.13482 (2)	0.01947 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0304 (8)	0.0241 (8)	0.0220 (8)	0.0019 (6)	-0.0012 (7)	-0.0029 (6)
C2	0.0336 (9)	0.0365 (9)	0.0204 (8)	0.0073 (7)	0.0003 (7)	0.0032 (7)
C3	0.0333 (9)	0.0288 (8)	0.0279 (9)	0.0083 (7)	0.0037 (7)	0.0103 (7)
C4	0.0307 (8)	0.0175 (7)	0.0308 (9)	0.0039 (6)	0.0037 (7)	0.0051 (6)
C5	0.0184 (6)	0.0152 (6)	0.0233 (7)	0.0020 (5)	0.0016 (6)	0.0006 (5)
C6	0.0178 (6)	0.0126 (6)	0.0237 (7)	-0.0008 (5)	0.0010 (5)	-0.0004 (5)
C7	0.0276 (8)	0.0130 (6)	0.0326 (9)	-0.0012 (6)	0.0015 (7)	-0.0030 (6)
C8	0.0293 (8)	0.0220 (7)	0.0334 (9)	-0.0058 (6)	0.0005 (7)	-0.0109 (7)
C9	0.0281 (8)	0.0286 (8)	0.0239 (8)	-0.0041 (6)	-0.0028 (6)	-0.0053 (6)

C10	0.0230 (7)	0.0215 (7)	0.0230 (8)	-0.0012 (6)	-0.0027 (6)	0.0001 (6)
N1	0.0219 (6)	0.0160 (5)	0.0209 (6)	0.0015 (5)	-0.0011 (5)	-0.0007 (5)
N2	0.0195 (6)	0.0139 (5)	0.0222 (6)	-0.0011 (4)	-0.0013 (5)	0.0000 (4)
O1W	0.0211 (5)	0.0150 (5)	0.0345 (7)	-0.0007 (4)	-0.0064 (5)	0.0023 (4)
O2W	0.0233 (6)	0.0193 (6)	0.0394 (7)	0.0001 (4)	-0.0027 (5)	-0.0115 (5)
O3	0.0356 (7)	0.0183 (6)	0.0527 (9)	0.0008 (5)	-0.0205 (6)	0.0035 (5)
O4	0.0308 (6)	0.0373 (7)	0.0398 (8)	-0.0013 (6)	-0.0138 (6)	-0.0121 (6)
O5	0.0461 (8)	0.0378 (8)	0.0386 (8)	-0.0010 (6)	0.0145 (7)	0.0068 (6)
O6	0.0275 (6)	0.0290 (6)	0.0379 (7)	-0.0014 (5)	0.0065 (5)	-0.0122 (5)
O7	0.0552 (9)	0.0157 (6)	0.0452 (8)	0.0009 (6)	-0.0055 (7)	-0.0011 (5)
O8	0.0338 (7)	0.0316 (6)	0.0302 (7)	-0.0026 (5)	-0.0140 (6)	-0.0030 (5)
O9	0.0221 (5)	0.0294 (6)	0.0254 (6)	-0.0003 (5)	0.0015 (5)	0.0040 (5)
O10	0.0187 (5)	0.0460 (8)	0.0325 (7)	0.0012 (5)	0.0009 (5)	0.0046 (6)
Cu1	0.02028 (10)	0.01089 (9)	0.02227 (10)	-0.00087 (6)	-0.00360 (7)	-0.00050 (6)
Cl1	0.02118 (16)	0.01651 (15)	0.02369 (18)	0.00116 (12)	-0.00293 (13)	-0.00168 (13)
Cl2	0.01900 (16)	0.01621 (15)	0.02290 (17)	-0.00066 (12)	-0.00351 (13)	0.00004 (12)

Geometric parameters (Å, °)

C1—N1	1.338 (2)	C10—N2	1.336 (2)
C1—C2	1.379 (2)	C10—H10	0.93
C1—H1	0.93	N1—Cu1	1.9723 (13)
C2—C3	1.376 (3)	N2—Cu1	1.9805 (12)
C2—H2	0.93	O1W—Cu1	1.9621 (12)
C3—C4	1.373 (3)	O2W—Cu1	1.9719 (12)
C3—H3	0.93	O1W—H1W	0.72 (2)
C4—C5	1.382 (2)	O1W—H2W	0.88 (2)
C4—H4	0.93	O2W—H3W	0.76 (2)
C5—N1	1.3432 (19)	O2W—H4W	0.78 (3)
C5—C6	1.469 (2)	O3—Cl1	1.4490 (12)
C6—N2	1.3448 (18)	O4—Cl1	1.4260 (12)
C6—C7	1.384 (2)	O5—Cl1	1.4236 (15)
C7—C8	1.374 (3)	O6—Cl1	1.4342 (13)
C7—H7	0.93	O7—Cl2	1.4217 (13)
C8—C9	1.376 (3)	O8—Cl2	1.4187 (12)
C8—H8	0.93	O9—Cl2	1.4503 (13)
C9—C10	1.382 (2)	O10—Cl2	1.4386 (12)
C9—H9	0.93	O9—Cu1	2.3287 (12)
N1—C1—C2	122.07 (16)	C10—N2—C6	119.10 (13)
N1—C1—H1	119	C10—N2—Cu1	126.53 (10)
C2—C1—H1	119	C6—N2—Cu1	114.28 (10)
C3—C2—C1	119.00 (16)	Cu1—O1W—H1W	113.8 (19)
C3—C2—H2	120.5	Cu1—O1W—H2W	117.2 (15)
C1—C2—H2	120.5	H1W—O1W—H2W	104 (2)
C4—C3—C2	119.23 (16)	Cu1—O2W—H3W	122.0 (19)
C4—C3—H3	120.4	Cu1—O2W—H4W	129.3 (17)
C2—C3—H3	120.4	H3W—O2W—H4W	104 (2)
C3—C4—C5	119.14 (16)	Cl2—O9—Cu1	130.08 (7)
C3—C4—H4	120.4	O1W—Cu1—O2W	91.60 (6)

supplementary materials

C5—C4—H4	120.4	O1W—Cu1—N1	169.24 (5)
N1—C5—C4	121.71 (15)	O2W—Cu1—N1	93.97 (6)
N1—C5—C6	114.64 (13)	O1W—Cu1—N2	93.62 (5)
C4—C5—C6	123.65 (14)	O2W—Cu1—N2	172.19 (5)
N2—C6—C7	121.64 (14)	N1—Cu1—N2	81.83 (6)
N2—C6—C5	114.61 (12)	O1W—Cu1—O9	91.11 (5)
C7—C6—C5	123.74 (14)	O2W—Cu1—O9	81.41 (5)
C8—C7—C6	118.94 (15)	N1—Cu1—O9	98.81 (5)
C8—C7—H7	120.5	N2—Cu1—O9	92.69 (5)
C6—C7—H7	120.5	O5—Cl1—O4	111.57 (9)
C7—C8—C9	119.45 (15)	O5—Cl1—O6	109.09 (9)
C7—C8—H8	120.3	O4—Cl1—O6	110.14 (8)
C9—C8—H8	120.3	O5—Cl1—O3	108.65 (9)
C8—C9—C10	118.96 (16)	O4—Cl1—O3	108.10 (8)
C8—C9—H9	120.5	O6—Cl1—O3	109.25 (9)
C10—C9—H9	120.5	O8—Cl2—O7	110.21 (8)
N2—C10—C9	121.87 (15)	O8—Cl2—O10	108.78 (8)
N2—C10—H10	119.1	O7—Cl2—O10	110.30 (9)
C9—C10—H10	119.1	O8—Cl2—O9	109.82 (8)
C1—N1—C5	118.84 (14)	O7—Cl2—O9	109.97 (9)
C1—N1—Cu1	126.52 (11)	O10—Cl2—O9	107.71 (7)
C5—N1—Cu1	114.59 (10)		
N1—C1—C2—C3	-0.6 (3)	C7—C6—N2—Cu1	-178.80 (12)
C1—C2—C3—C4	-0.3 (3)	C5—C6—N2—Cu1	0.18 (17)
C2—C3—C4—C5	0.7 (3)	C1—N1—Cu1—O1W	-113.5 (3)
C3—C4—C5—N1	-0.3 (3)	C5—N1—Cu1—O1W	63.8 (3)
C3—C4—C5—C6	179.30 (16)	C1—N1—Cu1—O2W	7.58 (15)
N1—C5—C6—N2	-1.7 (2)	C5—N1—Cu1—O2W	-175.14 (11)
C4—C5—C6—N2	178.72 (15)	C1—N1—Cu1—N2	-179.04 (15)
N1—C5—C6—C7	177.30 (15)	C5—N1—Cu1—N2	-1.76 (11)
C4—C5—C6—C7	-2.3 (3)	C1—N1—Cu1—O9	89.49 (14)
N2—C6—C7—C8	0.2 (3)	C5—N1—Cu1—O9	-93.24 (11)
C5—C6—C7—C8	-178.64 (16)	C10—N2—Cu1—O1W	13.96 (14)
C6—C7—C8—C9	1.1 (3)	C6—N2—Cu1—O1W	-169.38 (11)
C7—C8—C9—C10	-0.8 (3)	C10—N2—Cu1—N1	-175.84 (14)
C8—C9—C10—N2	-0.9 (3)	C6—N2—Cu1—N1	0.82 (11)
C2—C1—N1—C5	1.0 (3)	C10—N2—Cu1—O9	-77.32 (14)
C2—C1—N1—Cu1	178.17 (13)	C6—N2—Cu1—O9	99.34 (11)
C4—C5—N1—C1	-0.5 (2)	Cl2—O9—Cu1—O1W	-13.93 (10)
C6—C5—N1—C1	179.83 (14)	Cl2—O9—Cu1—O2W	-105.38 (10)
C4—C5—N1—Cu1	-178.04 (13)	Cl2—O9—Cu1—N1	161.89 (10)
C6—C5—N1—Cu1	2.33 (18)	Cl2—O9—Cu1—N2	79.74 (10)
C9—C10—N2—C6	2.2 (2)	Cu1—O9—Cl2—O8	-52.93 (12)
C9—C10—N2—Cu1	178.71 (12)	Cu1—O9—Cl2—O7	68.52 (11)
C7—C6—N2—C10	-1.9 (2)	Cu1—O9—Cl2—O10	-171.24 (9)
C5—C6—N2—C10	177.11 (14)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1W—H1W···O10 ⁱ	0.72 (2)	2.04 (2)	2.7078 (17)	155 (3)
O1W—H2W···O3 ⁱⁱ	0.88 (2)	1.89 (2)	2.7665 (17)	177.3 (18)
O2W—H3W···O3 ⁱⁱⁱ	0.76 (2)	2.13 (2)	2.8802 (18)	169 (2)
O2W—H4W···O4	0.78 (2)	2.37 (2)	2.9518 (19)	133 (2)
O2W—H4W···O7 ^{iv}	0.78 (2)	2.26 (3)	2.8349 (18)	132 (2)

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

supplementary materials

Fig. 1

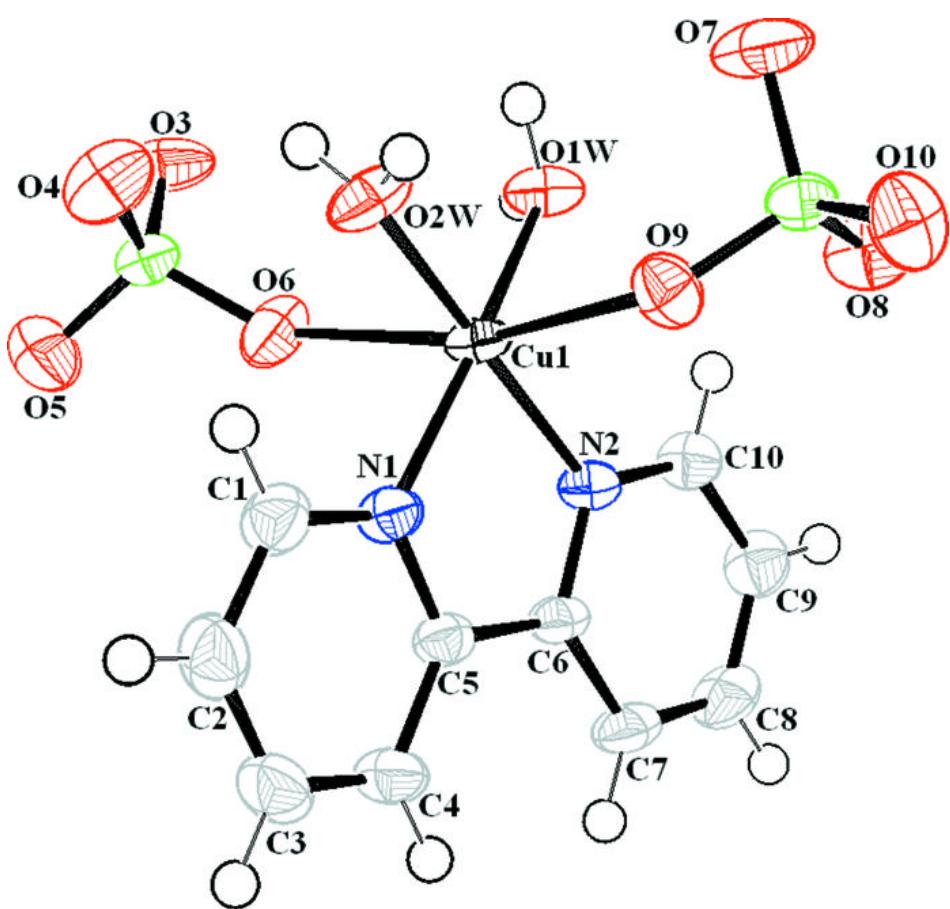
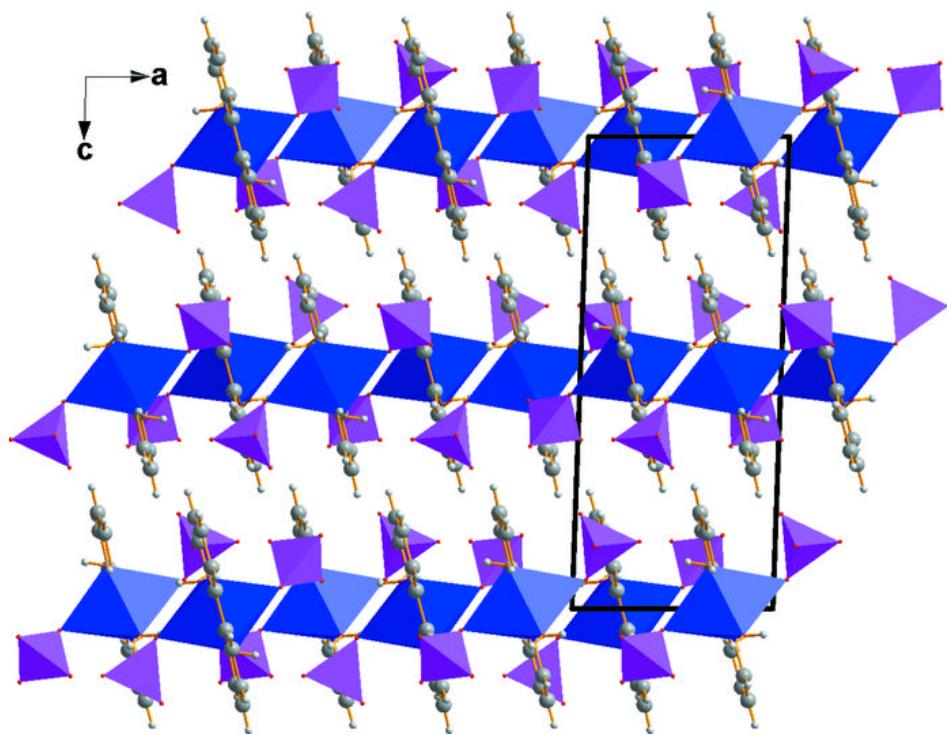


Fig. 2



supplementary materials

Fig. 3

