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Bis(acetato- κ^2O,O')(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')copper(II) monohydrate

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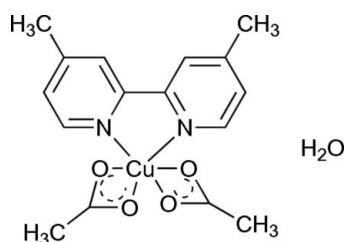
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.058; wR factor = 0.172; data-to-parameter ratio = 19.9.

In the title compound, $[Cu(C_2H_3O_2)_2(C_{12}H_{12}N_2)_2] \cdot H_2O$, the Cu^{II} atom exhibits a distorted octahedral coordination geometry, defined by two N atoms from one 4,4'-dimethyl-2,2'-bipyridine ligand and four O atoms from two acetate ligands. In the crystal, $O-H \cdots O$ hydrogen bonds are observed between the coordinated carboxylate O atoms and the solvent water molecule.

Related literature

For related structures, see: Willett *et al.* (2001); Amani *et al.* (2009); Hojjat Kashani *et al.* (2008); Alizadeh *et al.* (2009, 2010). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Cu(C_2H_3O_2)_2(C_{12}H_{12}N_2)_2] \cdot H_2O$
 $M_r = 383.88$
 Orthorhombic, *Pbcn*
 $a = 22.0667$ (8) Å
 $b = 9.0192$ (3) Å
 $c = 17.4088$ (6) Å
 $V = 3464.8$ (2) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 1.29$ mm⁻¹
 $T = 296$ K
 $0.48 \times 0.43 \times 0.26$ mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2008)
 $T_{min} = 0.544$, $T_{max} = 0.715$
 18193 measured reflections
 4559 independent reflections
 2835 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.091$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.172$
 $S = 1.00$
 4559 reflections
 229 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{max} = 0.46$ e Å⁻³
 $\Delta\rho_{min} = -0.87$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1S-H1S \cdots O4^i$	0.80 (6)	2.12 (6)	2.878 (4)	158 (5)
$O1S-H2S \cdots O11^{ii}$	0.91 (7)	2.19 (7)	2.876 (4)	132 (6)

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2130).

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supporting information

Acta Cryst. (2012). E68, m775 [doi:10.1107/S1600536812020193]

Bis(acetato- κ^2O,O')(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')copper(II) monohydrate

Aphiwat Kaewthong, Mongkol Sukwattanasinitt and Nongnuj Muangsin

S1. Comment

The transition metal complexes of 4,4'-dimethyl-2,2'-bipyridine (4,4'-dmbipy) with various secondary types of ligands have been reported, for example, copper with bromide (Willett *et al.*, 2001), iron with chloride (Amani *et al.*, 2009), platinum with chloride (Hojjat Kashani *et al.*, 2008), zinc with bromo (Alizadeh *et al.*, 2010) and zinc with iodide (Alizadeh *et al.*, 2009). Here, we report the title compound, $[\text{Cu}(\text{CH}_3\text{-bpy})(\text{OAc})_2]\cdot\text{H}_2\text{O}$, (I), a new copper complex with acetate ligands.

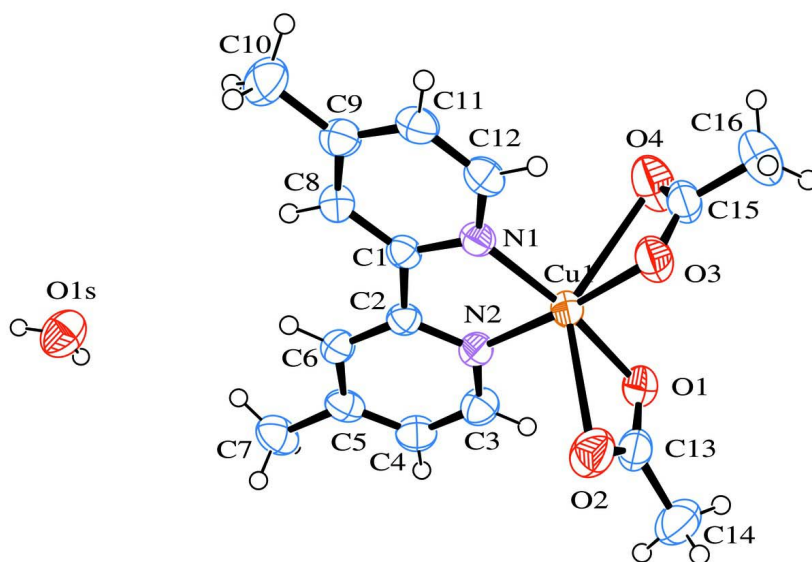
The asymmetric unit of the title compound, (I), is comprised of one water solvent molecule and a $[\text{Cu}(\text{CH}_3\text{-bpy})(\text{OAc})_2]$ complex with a distorted octahedral arrangement around the mononuclear copper (II) group as evidenced by bond angles of $\text{N1—Cu1—N2}[80.46(10)^\circ]$, $\text{N1—Cu1—O3}[94.27(9)^\circ]$, $\text{O1—Cu1—O3}[92.91(10)^\circ]$, $\text{O1—Cu1—N2}[92.41(9)^\circ]$. The six-coordinate geometry around the Cu (II) group is defined by two N atoms from one 4,4'-dimethyl-2,2'-bipyridine ligand and four O atoms from two acetate ligands. Bond lengths and angles are within normal ranges (Allen *et al.*, 1987). In the crystal structure, intermolecular $\text{O—H}\cdots\text{O}$ hydrogen bonds between the coordinated water molecules and the carboxylate O atoms may help stabilize the structure.

S2. Experimental

A solution of 4,4'-dimethyl-2,2'-bipyridine (17 mg, 0.1 mmol) and $\text{Cu}(\text{OAc})_2\cdot\text{H}_2\text{O}$ (20 mg, 0.1 mmol) in ethanol (10 ml) was stirred and refluxed for 2 h. The solution was placed for slow evaporation at room temperature, and after two weeks X-ray quality crystals of $\text{Cu}(\text{CH}_3\text{-bpy})(\text{OAc})_2$ appeared as blue prisms. Yield: 23 mg, 60%.

S3. Refinement

H1S and H2S were located by a difference map and refined isotropically. All the remaining H atoms were included in calculated positions, with C—H lengths fixed at 0.96 Å (CH₃) or 0.93 Å (CH). The isotropic displacement parameters for these atoms were set to 1.2 (CH) or 1.5 (CH₃) times U_{eq} of the parent atom.

**Figure 1**

Molecular structure of the title compound showing the atom labeling scheme of the asymmetric unit and 50% probability displacement ellipsoids.

Bis(acetato- κ^2O,O')(4,4'-dimethyl-2,2'-bipyridine- κ^2N,N')copper(II) monohydrate

Crystal data

$[\text{Cu}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_{12}\text{H}_{12}\text{N}_2)_2] \cdot \text{H}_2\text{O}$

$M_r = 383.88$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 22.0667$ (8) Å

$b = 9.0192$ (3) Å

$c = 17.4088$ (6) Å

$V = 3464.8$ (2) Å³

$Z = 8$

$F(000) = 1592$

$D_x = 1.472$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4435 reflections

$\theta = 2.3\text{--}27.3^\circ$

$\mu = 1.29$ mm⁻¹

$T = 296$ K

Prism, blue

$0.48 \times 0.43 \times 0.26$ mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer

Radiation source: sealed X-ray tube

Graphite monochromator

Detector resolution: 8.33 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2008)

$T_{\min} = 0.544$, $T_{\max} = 0.715$

18193 measured reflections

4559 independent reflections

2835 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.091$

$\theta_{\max} = 29.0^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -29 \rightarrow 27$

$k = -12 \rightarrow 12$

$l = -21 \rightarrow 23$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.172$
 $S = 1.00$
 4559 reflections
 229 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
 $w = 1/[\sigma^2(F_o^2) + (0.0896P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.014$
 $\Delta\rho_{\max} = 0.46 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.87 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. IR [KBr, cm^{-1}]: 3426, 3100, 1608, 1444, 1118, 770, 621. HRMS (ESI): m/z 389 $[M+\text{Na}]^+$.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.23138 (13)	0.3008 (3)	0.11076 (14)	0.0337 (6)
C2	0.25879 (12)	0.3929 (3)	0.04944 (14)	0.0339 (6)
C3	0.34865 (14)	0.4750 (3)	-0.00435 (16)	0.0448 (7)
H3	0.3908	0.4767	-0.0051	0.054*
C4	0.31721 (15)	0.5568 (3)	-0.05769 (16)	0.0456 (7)
H4	0.3384	0.6127	-0.0936	0.055*
C5	0.25498 (15)	0.5573 (3)	-0.05882 (14)	0.0412 (6)
C6	0.22514 (13)	0.4722 (3)	-0.00311 (15)	0.0379 (6)
H6	0.183	0.4693	-0.0016	0.046*
C7	0.21977 (17)	0.6439 (4)	-0.11742 (17)	0.0546 (9)
H7A	0.2403	0.7355	-0.1279	0.082*
H7B	0.18	0.6644	-0.0979	0.082*
H7C	0.2166	0.5871	-0.1639	0.082*
C8	0.17017 (14)	0.2973 (4)	0.12849 (15)	0.0404 (6)
H8	0.1434	0.3574	0.1015	0.049*
C9	0.14843 (14)	0.2055 (4)	0.18599 (17)	0.0428 (7)
C10	0.08269 (16)	0.2018 (5)	0.2063 (2)	0.0665 (10)
H10A	0.0642	0.2941	0.1921	0.1*
H10B	0.0783	0.1867	0.2606	0.1*
H10C	0.0633	0.1221	0.1792	0.1*
C11	0.19084 (14)	0.1170 (3)	0.22375 (16)	0.0421 (7)
H11	0.1782	0.0509	0.2615	0.051*
C12	0.25113 (14)	0.1271 (3)	0.20532 (16)	0.0422 (6)
H12	0.2787	0.0689	0.2323	0.051*
C13	0.44518 (14)	0.1966 (4)	0.02471 (18)	0.0472 (7)
C14	0.50052 (17)	0.2074 (5)	-0.0242 (2)	0.0669 (10)
H14A	0.5124	0.1101	-0.0407	0.1*

H14B	0.5328	0.2513	0.005	0.1*
H14C	0.492	0.2679	-0.0683	0.1*
C15	0.40175 (14)	0.1801 (4)	0.25884 (17)	0.0465 (7)
C16	0.4320 (2)	0.0955 (4)	0.3226 (2)	0.0695 (11)
H16A	0.4746	0.1167	0.3226	0.104*
H16B	0.4258	-0.0088	0.3151	0.104*
H16C	0.4148	0.1248	0.371	0.104*
N1	0.27219 (11)	0.2172 (3)	0.15003 (14)	0.0353 (5)
N2	0.32009 (11)	0.3924 (2)	0.04910 (12)	0.0369 (5)
O1	0.44010 (10)	0.2880 (3)	0.08035 (12)	0.0499 (5)
O1S	0.03896 (17)	1.0232 (4)	-0.12525 (17)	0.0744 (8)
H1S	0.062 (3)	1.080 (6)	-0.145 (3)	0.11 (2)*
H2S	0.003 (3)	1.064 (8)	-0.140 (4)	0.17 (3)*
O2	0.40469 (11)	0.1061 (3)	0.00996 (14)	0.0628 (6)
O3	0.38982 (10)	0.1081 (2)	0.19769 (12)	0.0512 (5)
O4	0.38908 (14)	0.3131 (3)	0.26600 (15)	0.0721 (8)
Cu1	0.359174 (16)	0.24915 (3)	0.122075 (19)	0.03621 (15)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0374 (15)	0.0331 (13)	0.0306 (12)	0.0006 (11)	-0.0018 (10)	-0.0027 (11)
C2	0.0383 (15)	0.0319 (13)	0.0315 (13)	0.0038 (10)	0.0012 (11)	-0.0039 (10)
C3	0.0423 (16)	0.0437 (16)	0.0482 (17)	-0.0031 (13)	0.0049 (13)	0.0047 (13)
C4	0.0516 (19)	0.0430 (17)	0.0422 (15)	-0.0043 (12)	0.0065 (13)	0.0064 (12)
C5	0.0577 (19)	0.0337 (14)	0.0321 (13)	0.0085 (11)	0.0003 (13)	-0.0005 (11)
C6	0.0361 (15)	0.0401 (15)	0.0376 (14)	0.0067 (11)	0.0016 (11)	-0.0004 (12)
C7	0.072 (2)	0.0497 (19)	0.0425 (17)	0.0115 (16)	-0.0060 (14)	0.0082 (14)
C8	0.0360 (16)	0.0460 (15)	0.0393 (15)	0.0019 (13)	-0.0026 (12)	-0.0010 (12)
C9	0.0431 (17)	0.0462 (15)	0.0392 (16)	-0.0104 (12)	0.0023 (12)	-0.0018 (13)
C10	0.042 (2)	0.088 (3)	0.070 (2)	-0.0099 (18)	0.0070 (17)	0.019 (2)
C11	0.0495 (18)	0.0436 (16)	0.0332 (13)	-0.0080 (13)	0.0008 (12)	0.0018 (12)
C12	0.0500 (18)	0.0403 (15)	0.0362 (14)	0.0007 (12)	-0.0036 (13)	0.0051 (11)
C13	0.0342 (16)	0.0573 (18)	0.0501 (17)	0.0060 (14)	-0.0013 (13)	0.0084 (15)
C14	0.050 (2)	0.079 (2)	0.072 (2)	0.0076 (18)	0.0164 (18)	0.008 (2)
C15	0.0403 (17)	0.056 (2)	0.0436 (16)	0.0002 (14)	-0.0090 (13)	0.0072 (14)
C16	0.077 (3)	0.072 (2)	0.060 (2)	0.0003 (19)	-0.0247 (19)	0.0156 (19)
N1	0.0384 (13)	0.0371 (12)	0.0305 (11)	0.0022 (9)	-0.0003 (10)	0.0011 (9)
N2	0.0348 (12)	0.0389 (12)	0.0371 (12)	0.0010 (9)	0.0012 (9)	0.0013 (10)
O1	0.0354 (12)	0.0657 (13)	0.0487 (13)	0.0004 (10)	-0.0037 (9)	0.0006 (11)
O1S	0.065 (2)	0.0660 (18)	0.092 (2)	0.0099 (15)	0.0102 (16)	0.0145 (16)
O2	0.0445 (13)	0.0694 (16)	0.0743 (16)	-0.0041 (11)	0.0014 (12)	-0.0130 (12)
O3	0.0515 (13)	0.0535 (13)	0.0486 (12)	0.0073 (10)	-0.0124 (10)	0.0020 (10)
O4	0.087 (2)	0.0588 (15)	0.0709 (16)	0.0163 (15)	-0.0301 (14)	-0.0092 (14)
Cu1	0.0334 (2)	0.0398 (3)	0.0354 (2)	0.00240 (13)	-0.00412 (13)	-0.00033 (13)

Geometric parameters (Å, °)

C1—N1	1.359 (4)	C11—C12	1.372 (4)
C1—C8	1.386 (4)	C11—H11	0.93
C1—C2	1.482 (4)	C12—N1	1.343 (4)
C2—N2	1.353 (3)	C12—H12	0.93
C2—C6	1.378 (4)	C13—O2	1.237 (4)
C3—N2	1.349 (3)	C13—O1	1.277 (4)
C3—C4	1.374 (4)	C13—C14	1.492 (5)
C3—H3	0.93	C14—H14A	0.96
C4—C5	1.373 (5)	C14—H14B	0.96
C4—H4	0.93	C14—H14C	0.96
C5—C6	1.401 (4)	C15—O4	1.238 (4)
C5—C7	1.501 (4)	C15—O3	1.275 (4)
C6—H6	0.93	C15—C16	1.504 (4)
C7—H7A	0.96	C16—H16A	0.96
C7—H7B	0.96	C16—H16B	0.96
C7—H7C	0.96	C16—H16C	0.96
C8—C9	1.385 (4)	N1—Cu1	2.001 (2)
C8—H8	0.93	N2—Cu1	2.007 (2)
C9—C11	1.395 (4)	O1—Cu1	1.959 (2)
C9—C10	1.493 (5)	O1S—H1S	0.80 (6)
C10—H10A	0.96	O1S—H2S	0.91 (7)
C10—H10B	0.96	O3—Cu1	1.952 (2)
C10—H10C	0.96		
N1—C1—C8	121.4 (3)	C9—C11—H11	119.9
N1—C1—C2	113.8 (2)	N1—C12—C11	122.9 (3)
C8—C1—C2	124.8 (3)	N1—C12—H12	118.5
N2—C2—C6	122.5 (2)	C11—C12—H12	118.5
N2—C2—C1	114.2 (2)	O2—C13—O1	121.3 (3)
C6—C2—C1	123.3 (3)	O2—C13—C14	121.1 (3)
N2—C3—C4	121.8 (3)	O1—C13—C14	117.5 (3)
N2—C3—H3	119.1	C13—C14—H14A	109.5
C4—C3—H3	119.1	C13—C14—H14B	109.5
C5—C4—C3	121.1 (3)	H14A—C14—H14B	109.5
C5—C4—H4	119.4	C13—C14—H14C	109.5
C3—C4—H4	119.4	H14A—C14—H14C	109.5
C4—C5—C6	117.3 (2)	H14B—C14—H14C	109.5
C4—C5—C7	121.9 (3)	O4—C15—O3	122.1 (3)
C6—C5—C7	120.8 (3)	O4—C15—C16	121.2 (3)
C2—C6—C5	119.4 (3)	O3—C15—C16	116.8 (3)
C2—C6—H6	120.3	C15—C16—H16A	109.5
C5—C6—H6	120.3	C15—C16—H16B	109.5
C5—C7—H7A	109.5	H16A—C16—H16B	109.5
C5—C7—H7B	109.5	C15—C16—H16C	109.5
H7A—C7—H7B	109.5	H16A—C16—H16C	109.5
C5—C7—H7C	109.5	H16B—C16—H16C	109.5

H7A—C7—H7C	109.5	C12—N1—C1	117.9 (3)
H7B—C7—H7C	109.5	C12—N1—Cu1	126.4 (2)
C9—C8—C1	120.8 (3)	C1—N1—Cu1	115.70 (19)
C9—C8—H8	119.6	C3—N2—C2	117.9 (2)
C1—C8—H8	119.6	C3—N2—Cu1	126.3 (2)
C8—C9—C11	116.8 (3)	C2—N2—Cu1	115.43 (16)
C8—C9—C10	121.4 (3)	C13—O1—Cu1	104.23 (19)
C11—C9—C10	121.8 (3)	H1S—O1S—H2S	100 (5)
C9—C10—H10A	109.5	C15—O3—Cu1	107.6 (2)
C9—C10—H10B	109.5	O3—Cu1—O1	92.91 (10)
H10A—C10—H10B	109.5	O3—Cu1—N1	94.27 (9)
C9—C10—H10C	109.5	O1—Cu1—N1	171.94 (9)
H10A—C10—H10C	109.5	O3—Cu1—N2	174.64 (9)
H10B—C10—H10C	109.5	O1—Cu1—N2	92.41 (9)
C12—C11—C9	120.2 (3)	N1—Cu1—N2	80.46 (10)
C12—C11—H11	119.9		
N1—C1—C2—N2	-7.7 (3)	C2—C1—N1—Cu1	4.5 (3)
C8—C1—C2—N2	172.0 (3)	C4—C3—N2—C2	-0.6 (4)
N1—C1—C2—C6	172.1 (2)	C4—C3—N2—Cu1	172.2 (2)
C8—C1—C2—C6	-8.2 (4)	C6—C2—N2—C3	1.0 (4)
N2—C3—C4—C5	-0.2 (4)	C1—C2—N2—C3	-179.2 (2)
C3—C4—C5—C6	0.5 (4)	C6—C2—N2—Cu1	-172.5 (2)
C3—C4—C5—C7	-179.0 (3)	C1—C2—N2—Cu1	7.3 (3)
N2—C2—C6—C5	-0.7 (4)	O2—C13—O1—Cu1	-2.6 (4)
C1—C2—C6—C5	179.5 (2)	C14—C13—O1—Cu1	174.6 (3)
C4—C5—C6—C2	-0.1 (4)	O4—C15—O3—Cu1	6.1 (4)
C7—C5—C6—C2	179.4 (3)	C16—C15—O3—Cu1	-174.1 (3)
N1—C1—C8—C9	-1.5 (4)	C15—O3—Cu1—O1	90.9 (2)
C2—C1—C8—C9	178.8 (3)	C15—O3—Cu1—N1	-92.8 (2)
C1—C8—C9—C11	-0.7 (4)	C13—O1—Cu1—O3	92.8 (2)
C1—C8—C9—C10	179.4 (3)	C13—O1—Cu1—N2	-87.8 (2)
C8—C9—C11—C12	2.3 (4)	C12—N1—Cu1—O3	1.4 (2)
C10—C9—C11—C12	-177.8 (3)	C1—N1—Cu1—O3	178.4 (2)
C9—C11—C12—N1	-1.8 (4)	C12—N1—Cu1—N2	-177.6 (2)
C11—C12—N1—C1	-0.4 (4)	C1—N1—Cu1—N2	-0.6 (2)
C11—C12—N1—Cu1	176.5 (2)	C3—N2—Cu1—O1	-0.5 (2)
C8—C1—N1—C12	2.1 (4)	C2—N2—Cu1—O1	172.35 (18)
C2—C1—N1—C12	-178.2 (2)	C3—N2—Cu1—N1	-176.8 (2)
C8—C1—N1—Cu1	-175.2 (2)	C2—N2—Cu1—N1	-3.87 (18)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1S—H1S \cdots O4 ⁱ	0.80 (6)	2.12 (6)	2.878 (4)	158 (5)
O1S—H2S \cdots O1 ⁱⁱ	0.91 (7)	2.19 (7)	2.876 (4)	132 (6)

Symmetry codes: (i) $-x+1/2, -y+3/2, z-1/2$; (ii) $x-1/2, -y+3/2, -z$.