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Poly[[bis(acetonitrile- κ N)bis[μ -2,2'-(methylenedithio)bis(1,3,4-thiadiazole)- κ^2 N⁴:N^{4'}]]copper(II)] bis(perchlorate) acetonitrile solvate]

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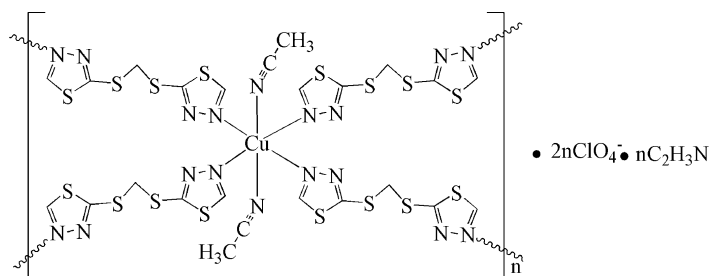
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 Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.015$ Å; disorder in solvent or counterion; R factor = 0.057; wR factor = 0.181; data-to-parameter ratio = 15.2.

In the title compound, $\{[\text{Cu}(\text{C}_5\text{H}_4\text{N}_4\text{S}_4)_2(\text{C}_2\text{H}_3\text{N})_2](\text{ClO}_4)_2 \cdot n\text{C}_2\text{H}_3\text{N}\}_m$, the Cu^{II} atom occupies a crystallographic inversion centre and is six-coordinated by six N atoms of four symmetry-related 2,2'-(methylenedithio)bis(1,3,4-thiadiazole) (L) ligands and two acetonitrile molecules in a slightly distorted octahedral geometry. The ligand L adopts an $N:N'$ -bidentate bridging mode in a *trans* configuration, bridging the Cu atoms *via* translation symmetry, forming a two-dimensional layer-like structure. The perchlorate ions serve as acceptors for intermolecular $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds, which link the layers into a three-dimensional network. The ClO_4^- anion is disordered with an occupation ratio of 0.658:0.342.

Related literature

For literature on Cu–N bonds, see: Huang *et al.* (2009); Qin *et al.* (2009); Wang *et al.* (2008).



Experimental

Crystal data

$[\text{Cu}(\text{C}_5\text{H}_4\text{N}_4\text{S}_4)_2(\text{C}_2\text{H}_3\text{N})_2](\text{ClO}_4)_2 \cdot n\text{C}_2\text{H}_3\text{N}$
 $M_r = 1764.65$
 Monoclinic, $C2/c$
 $a = 19.3144$ (18) Å
 $b = 9.9450$ (9) Å
 $c = 18.8722$ (18) Å
 $\beta = 98.876$ (1) $^\circ$
 $V = 3581.6$ (6) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.28$ mm⁻¹
 $T = 294$ K
 $0.43 \times 0.32 \times 0.30$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
 $T_{\text{min}} = 0.608$, $T_{\text{max}} = 0.702$
 12066 measured reflections
 3285 independent reflections
 2568 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.181$
 $S = 1.07$
 3285 reflections
 216 parameters
 304 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.86$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.83$ e Å⁻³

Table 1

 Hydrogen-bond geometry (Å, $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{C1}-\text{H1} \cdots \text{O3}^{\text{i}}$	0.93	2.35	2.955 (8)	123
$\text{C3}-\text{H3A} \cdots \text{O1}^{\text{ii}}$	0.97	2.41	3.277 (9)	149
$\text{C5}-\text{H5} \cdots \text{O1}^{\text{iii}}$	0.93	2.45	3.169 (9)	135

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank Luoyang Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2101).

References

- Bruker (1997). *SMART*, *SAINTE* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Huang, H.-M., Ju, F.-Y., Wang, J.-G. & Qin, J.-H. (2009). *Acta Cryst.* **E65**, m80–m81.
 Qin, J.-H., Wang, J.-G. & Hu, P.-Z. (2009). *Acta Cryst.* **E65**, m349–m350.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Wang, J. G., Qin, J. H., Hu, P. Z. & Zhao, B. T. (2008). *Z. Kristallogr. New Cryst. Struct.* **223**, 225–227.

supporting information

Acta Cryst. (2009). E65, m415 [doi:10.1107/S1600536809008708]

Poly[[bis(acetonitrile- κ N)bis[μ_2 -2,2'-(methylenedithio)bis(1,3,4-thiadiazole)- κ^2 N⁴:N^{4'}]]copper(II)] bis(perchlorate) acetonitrile solvate]

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S1. Comment

The asymmetric unit of the title compound consists of half a Cu^{II} atom, two independent 2,2'-(methylenedithio)bis(1,3,4-thiadiazole) (*L*) ligands, one coordinated acetonitrile molecule, one uncoordinated acetonitrile molecule, and one perchlorate ion (Fig. 1). The Cu^{II} atom is coordinated by six N atoms, from four *L* ligands and two acetonitrile molecules, in a slightly distorted octahedral geometry. All six Cu—N bond distances are within the range expected for such coordination bonds (Huang *et al.*, 2009; Wang *et al.*, 2008; Qin *et al.*, 2009). The ligand *L* adopts a *N*:*N'*-bidentate bridging mode in *trans* configuration, so bridging the copper atoms *via* translation symmetry to form a two-dimensional layer-like structure, with a bridging Cu...Cu distance of 10.6661 (8) Å (Fig. 2). The centroid-centroid separation and dihedral angle of the thiadiazole rings are 6.3928 (5) Å and 81.86 (13)°, respectively.

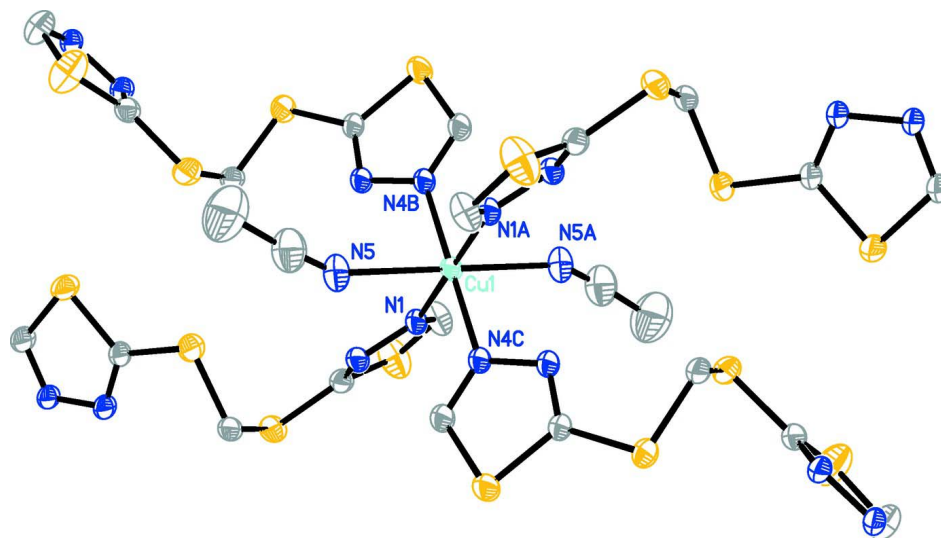
In the crystal structure the region between the layers is taken up by perchlorate ions and uncoordinated acetonitrile molecules. The perchlorate ions serve as acceptors for C—H...O hydrogen-bonds, which link the chains into a three-dimensional network (Table 1 and Fig. 3).

S2. Experimental

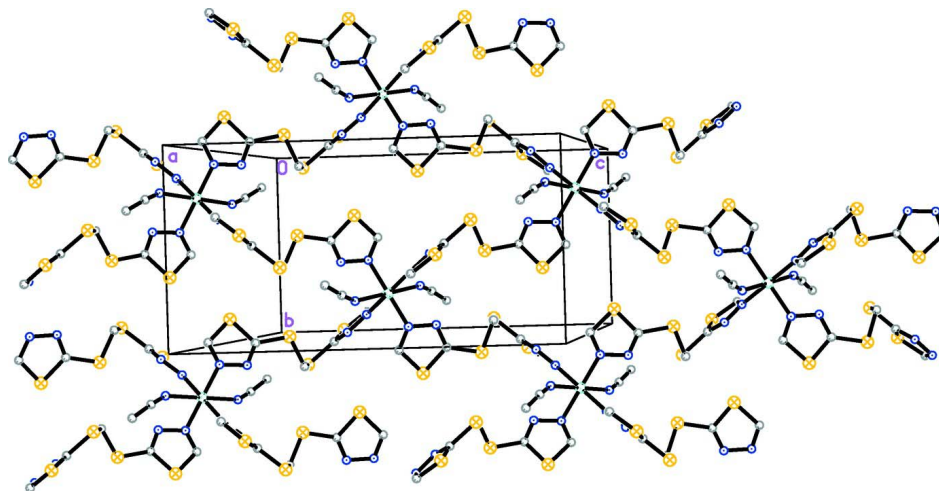
The reaction of 2,2'-(methylenedithio)bis(1,3,4-thiadiazole) (0.2 mmol) with Cu(ClO₄)₂ (0.1 mmol) in an acetonitrile solution (20 ml) afforded a light blue solid after a few minutes. It was filtered off, washed with acetone, and dried in air. Single crystals, suitable for X-ray analysis, were obtained by slow diffusion of Et₂O into an acetonitrile solution of the solid.

S3. Refinement

All H-atoms were positioned geometrically and treated as riding: C—H = 0.93 - 09.7 Å with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{parent C-atom})$.

**Figure 1**

A view of the molecular structure of the cation in the title compound. Displacement ellipsoids are drawn at the 30% probability level. The H atoms, perchlorate ion, and uncoordinated acetonitrile molecules were omitted for clarity [symmetry operations: A: $1/2-x, 3/2-y, -z$; B: $1/2-x, -1/2+y, 1/2-z$; C: $x, 2-y, -1/2+z$].

**Figure 2**

A view of the two-dimensional network in the title compound.

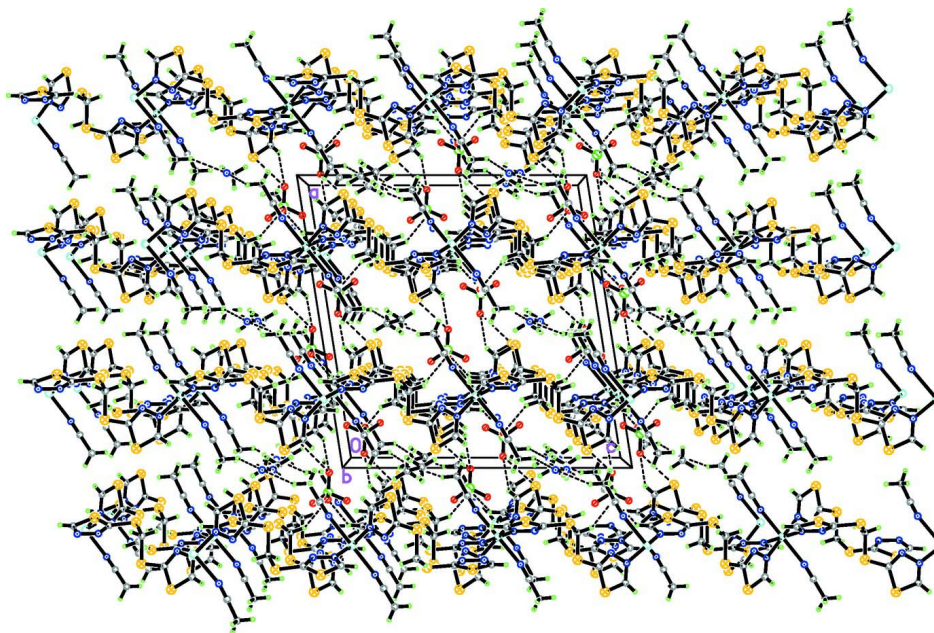


Figure 3

A view down the b axis of the crystal packing of the title compound.

Poly[[bis(acetonitrile- κ N)bis[μ -2,2'-(methylenedithio)bis(1,3,4-thiadiazole)- κ^2 N⁴:N⁴]]copper(II)] bis(perchlorate) acetonitrile solvate]

Crystal data

[Cu(C₅H₄N₄S₄)₂(C₂H₃N)₂](ClO₄)₂·C₂H₃N

$M_r = 1764.65$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 19.3144\ (18)\ \text{\AA}$

$b = 9.9450\ (9)\ \text{\AA}$

$c = 18.8722\ (18)\ \text{\AA}$

$\beta = 98.876\ (1)^\circ$

$V = 3581.6\ (6)\ \text{\AA}^3$

$Z = 2$

$F(000) = 1780$

$D_x = 1.636\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5001 reflections

$\theta = 2.3\text{--}28.0^\circ$

$\mu = 1.28\ \text{mm}^{-1}$

$T = 294\ \text{K}$

Block, blue

$0.43 \times 0.32 \times 0.30\ \text{mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 1997)

$T_{\min} = 0.608$, $T_{\max} = 0.702$

12066 measured reflections

3285 independent reflections

2568 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -23 \rightarrow 23$

$k = -12 \rightarrow 12$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.181$

$S = 1.07$

3285 reflections

216 parameters

304 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1007P)^2 + 13.6762P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.86 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.83 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C11	0.40159 (11)	0.1887 (3)	0.92446 (12)	0.1040 (7)	0.658 (6)
O1	0.3842 (4)	0.3266 (6)	0.9249 (4)	0.135 (2)	0.658 (6)
O2	0.3626 (4)	0.1399 (7)	0.8620 (4)	0.146 (3)	0.658 (6)
O3	0.4718 (3)	0.1679 (9)	0.9382 (4)	0.139 (2)	0.658 (6)
O4	0.3720 (5)	0.1390 (8)	0.9838 (4)	0.150 (3)	0.658 (6)
C11'	0.40159 (11)	0.1887 (3)	0.92446 (12)	0.1040 (7)	0.342 (6)
O1'	0.3333 (3)	0.2118 (9)	0.9325 (5)	0.135 (2)	0.342 (6)
O2'	0.4400 (4)	0.0929 (7)	0.9670 (4)	0.146 (3)	0.342 (6)
O3'	0.4391 (4)	0.3116 (7)	0.9371 (5)	0.139 (2)	0.342 (6)
O4'	0.4083 (5)	0.1678 (8)	0.8518 (3)	0.150 (3)	0.342 (6)
Cu1	0.2500	0.7500	0.0000	0.0403 (3)	
S1	0.41916 (9)	0.9410 (2)	0.16187 (11)	0.0858 (6)	
S2	0.32021 (8)	1.10571 (14)	0.23555 (7)	0.0551 (4)	
S3	0.18788 (8)	0.94899 (14)	0.24653 (6)	0.0542 (4)	
S4	0.17640 (9)	0.85456 (14)	0.39769 (7)	0.0584 (4)	
N1	0.3156 (2)	0.8589 (4)	0.07448 (19)	0.0424 (9)	
N2	0.2872 (2)	0.9444 (4)	0.12019 (19)	0.0421 (9)	
N3	0.2193 (2)	1.0883 (4)	0.36936 (19)	0.0445 (9)	
N4	0.2208 (2)	1.0822 (4)	0.44266 (19)	0.0425 (9)	
N5	0.1534 (3)	0.7792 (6)	0.0641 (3)	0.0662 (13)	
C1	0.3821 (3)	0.8491 (7)	0.0899 (3)	0.0651 (16)	
H1	0.4084	0.7955	0.0637	0.078*	
C2	0.3356 (3)	0.9939 (5)	0.1685 (2)	0.0454 (11)	
C3	0.2265 (3)	1.1032 (5)	0.2201 (3)	0.0498 (12)	
H3A	0.2105	1.1181	0.1694	0.060*	
H3B	0.2095	1.1773	0.2461	0.060*	
C4	0.1974 (3)	0.9770 (5)	0.3392 (2)	0.0410 (10)	
C5	0.1996 (3)	0.9686 (5)	0.4642 (3)	0.0509 (13)	
H5	0.1973	0.9505	0.5121	0.061*	
C6	0.1050 (4)	0.7464 (9)	0.0852 (4)	0.088 (2)	
C7	0.0400 (6)	0.6925 (15)	0.1112 (7)	0.144 (4)	
H7A	-0.0006	0.7375	0.0865	0.216*	
H7B	0.0434	0.7083	0.1618	0.216*	
H7C	0.0361	0.5977	0.1019	0.216*	

N6	1.000 (2)	-0.171 (2)	0.2314 (17)	0.212 (10)	0.50
C8	0.9970 (14)	-0.059 (2)	0.2284 (11)	0.208 (11)	0.50
C9	0.993 (2)	0.093 (2)	0.2242 (18)	0.204 (11)	0.50
H9A	1.0400	0.1296	0.2300	0.306*	0.50
H9B	0.9696	0.1270	0.2617	0.306*	0.50
H9C	0.9682	0.1199	0.1785	0.306*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0787 (12)	0.1298 (17)	0.0987 (14)	0.0298 (12)	-0.0016 (10)	-0.0166 (13)
O1	0.118 (4)	0.147 (4)	0.137 (4)	0.040 (4)	0.012 (4)	-0.018 (4)
O2	0.136 (5)	0.150 (4)	0.141 (4)	0.019 (4)	-0.016 (4)	-0.013 (4)
O3	0.105 (4)	0.156 (4)	0.156 (5)	0.017 (4)	0.018 (4)	-0.001 (4)
O4	0.141 (5)	0.173 (5)	0.138 (4)	0.009 (4)	0.036 (4)	0.000 (4)
C11'	0.0787 (12)	0.1298 (17)	0.0987 (14)	0.0298 (12)	-0.0016 (10)	-0.0166 (13)
O1'	0.118 (4)	0.147 (4)	0.137 (4)	0.040 (4)	0.012 (4)	-0.018 (4)
O2'	0.136 (5)	0.150 (4)	0.141 (4)	0.019 (4)	-0.016 (4)	-0.013 (4)
O3'	0.105 (4)	0.156 (4)	0.156 (5)	0.017 (4)	0.018 (4)	-0.001 (4)
O4'	0.141 (5)	0.173 (5)	0.138 (4)	0.009 (4)	0.036 (4)	0.000 (4)
Cu1	0.0650 (6)	0.0348 (4)	0.0214 (4)	0.0057 (3)	0.0075 (3)	-0.0001 (3)
S1	0.0569 (9)	0.1161 (16)	0.0808 (12)	0.0020 (9)	-0.0006 (8)	-0.0383 (11)
S2	0.0796 (9)	0.0467 (7)	0.0378 (7)	-0.0078 (6)	0.0053 (6)	-0.0117 (5)
S3	0.0840 (10)	0.0491 (7)	0.0300 (6)	-0.0130 (6)	0.0106 (6)	-0.0096 (5)
S4	0.0932 (11)	0.0443 (7)	0.0401 (7)	-0.0216 (7)	0.0176 (7)	-0.0046 (5)
N1	0.058 (3)	0.042 (2)	0.0291 (18)	0.0056 (18)	0.0118 (17)	0.0004 (16)
N2	0.058 (2)	0.039 (2)	0.0292 (18)	0.0026 (18)	0.0076 (17)	-0.0023 (15)
N3	0.067 (3)	0.041 (2)	0.0275 (18)	-0.0069 (19)	0.0127 (17)	-0.0023 (16)
N4	0.064 (3)	0.040 (2)	0.0253 (18)	-0.0051 (18)	0.0104 (17)	-0.0005 (15)
N5	0.072 (3)	0.082 (3)	0.049 (3)	0.001 (3)	0.022 (2)	-0.006 (2)
C1	0.061 (4)	0.078 (4)	0.057 (3)	0.007 (3)	0.011 (3)	-0.020 (3)
C2	0.063 (3)	0.040 (2)	0.033 (2)	-0.002 (2)	0.007 (2)	0.0015 (19)
C3	0.085 (4)	0.037 (2)	0.029 (2)	0.006 (2)	0.013 (2)	-0.0002 (19)
C4	0.054 (3)	0.041 (2)	0.029 (2)	-0.003 (2)	0.0103 (19)	-0.0025 (19)
C5	0.078 (4)	0.046 (3)	0.030 (2)	-0.011 (3)	0.013 (2)	-0.004 (2)
C6	0.085 (4)	0.112 (5)	0.066 (4)	-0.001 (4)	0.012 (3)	-0.008 (3)
C7	0.116 (6)	0.184 (8)	0.138 (7)	-0.028 (6)	0.037 (5)	0.012 (7)
N6	0.208 (12)	0.212 (11)	0.217 (14)	-0.002 (10)	0.033 (10)	0.002 (9)
C8	0.202 (12)	0.209 (12)	0.213 (14)	0.002 (9)	0.030 (9)	0.003 (9)
C9	0.197 (14)	0.205 (12)	0.211 (15)	0.003 (10)	0.036 (10)	0.002 (9)

Geometric parameters (Å, °)

C11—O3	1.356 (5)	N1—C1	1.277 (8)
C11—O2	1.385 (5)	N1—N2	1.382 (5)
C11—O1	1.411 (5)	N2—C2	1.298 (6)
C11—O4	1.422 (5)	N3—C4	1.286 (6)
C11'—O1'	1.371 (5)	N3—N4	1.380 (5)

C11'—O2'	1.385 (5)	N4—C5	1.288 (6)
C11'—O4'	1.413 (5)	N4—Cu1 ^{iv}	2.021 (4)
C11'—O3'	1.422 (5)	N5—C6	1.119 (8)
Cu1—N4 ⁱ	2.021 (4)	C1—H1	0.9300
Cu1—N4 ⁱⁱ	2.021 (4)	C3—H3A	0.9700
Cu1—N1 ⁱⁱⁱ	2.050 (4)	C3—H3B	0.9700
Cu1—N1	2.050 (4)	C5—H5	0.9300
Cu1—N5 ⁱⁱⁱ	2.393 (5)	C6—C7	1.515 (11)
Cu1—N5	2.393 (5)	C7—H7A	0.9600
S1—C1	1.700 (6)	C7—H7B	0.9600
S1—C2	1.720 (6)	C7—H7C	0.9600
S2—C2	1.744 (5)	N6—C8	1.114 (6)
S2—C3	1.789 (6)	C8—C9	1.523 (8)
S3—C4	1.752 (4)	C9—H9A	0.9600
S3—C3	1.809 (5)	C9—H9B	0.9600
S4—C5	1.699 (5)	C9—H9C	0.9600
S4—C4	1.734 (5)		
O3—C11—O2	120.3	N2—N1—Cu1	119.4 (3)
O3—C11—O1	112.3	C2—N2—N1	111.1 (4)
O2—C11—O1	104.3	C4—N3—N4	111.1 (4)
O3—C11—O4	107.9	C5—N4—N3	113.3 (4)
O2—C11—O4	108.5	C5—N4—Cu1 ^{iv}	129.1 (3)
O1—C11—O4	102.0	N3—N4—Cu1 ^{iv}	117.5 (3)
O1'—C11'—O2'	119.3	C6—N5—Cu1	154.6 (6)
O1'—C11'—O4'	111.4	N1—C1—S1	115.2 (4)
O2'—C11'—O4'	109.9	N1—C1—H1	122.4
O1'—C11'—O3'	108.2	S1—C1—H1	122.4
O2'—C11'—O3'	106.3	N2—C2—S1	114.5 (4)
O4'—C11'—O3'	99.7	N2—C2—S2	124.6 (4)
N4 ⁱ —Cu1—N4 ⁱⁱ	180.0	S1—C2—S2	121.0 (3)
N4 ⁱ —Cu1—N1 ⁱⁱⁱ	91.30 (15)	S2—C3—S3	114.6 (3)
N4 ⁱⁱ —Cu1—N1 ⁱⁱⁱ	88.70 (15)	S2—C3—H3A	108.6
N4 ⁱ —Cu1—N1	88.70 (15)	S3—C3—H3A	108.6
N4 ⁱⁱ —Cu1—N1	91.30 (15)	S2—C3—H3B	108.6
N1 ⁱⁱⁱ —Cu1—N1	180.0	S3—C3—H3B	108.6
N4 ⁱ —Cu1—N5 ⁱⁱⁱ	89.75 (18)	H3A—C3—H3B	107.6
N4 ⁱⁱ —Cu1—N5 ⁱⁱⁱ	90.25 (18)	N3—C4—S4	114.6 (3)
N1 ⁱⁱⁱ —Cu1—N5 ⁱⁱⁱ	92.10 (17)	N3—C4—S3	123.8 (3)
N1—Cu1—N5 ⁱⁱⁱ	87.90 (17)	S4—C4—S3	121.7 (3)
N4 ⁱ —Cu1—N5	90.25 (18)	N4—C5—S4	114.4 (4)
N4 ⁱⁱ —Cu1—N5	89.75 (18)	N4—C5—H5	122.8
N1 ⁱⁱⁱ —Cu1—N5	87.90 (17)	S4—C5—H5	122.8
N1—Cu1—N5	92.10 (17)	N5—C6—C7	176.0 (10)
N5 ⁱⁱⁱ —Cu1—N5	180.0	C6—C7—H7A	109.5
C1—S1—C2	86.5 (3)	C6—C7—H7B	109.5
C2—S2—C3	98.9 (2)	H7A—C7—H7B	109.5
C4—S3—C3	99.0 (2)	C6—C7—H7C	109.5

C5—S4—C4	86.6 (2)	H7A—C7—H7C	109.5
C1—N1—N2	112.7 (4)	H7B—C7—H7C	109.5
C1—N1—Cu1	127.6 (4)	N6—C8—C9	180.0
N4 ⁱ —Cu1—N1—C1	63.0 (5)	C2—S1—C1—N1	-0.1 (5)
N4 ⁱⁱ —Cu1—N1—C1	-117.0 (5)	N1—N2—C2—S1	0.3 (5)
N5 ⁱⁱⁱ —Cu1—N1—C1	-26.8 (5)	N1—N2—C2—S2	179.9 (3)
N5—Cu1—N1—C1	153.2 (5)	C1—S1—C2—N2	-0.1 (4)
N4 ⁱ —Cu1—N1—N2	-109.4 (3)	C1—S1—C2—S2	-179.8 (4)
N4 ⁱⁱ —Cu1—N1—N2	70.6 (3)	C3—S2—C2—N2	6.9 (5)
N5 ⁱⁱⁱ —Cu1—N1—N2	160.8 (3)	C3—S2—C2—S1	-173.5 (3)
N5—Cu1—N1—N2	-19.2 (3)	C2—S2—C3—S3	71.7 (3)
C1—N1—N2—C2	-0.4 (6)	C4—S3—C3—S2	78.6 (3)
Cu1—N1—N2—C2	173.1 (3)	N4—N3—C4—S4	0.2 (5)
C4—N3—N4—C5	-0.6 (6)	N4—N3—C4—S3	179.3 (4)
C4—N3—N4—Cu1 ^{iv}	-177.6 (3)	C5—S4—C4—N3	0.2 (4)
N4 ⁱ —Cu1—N5—C6	-53.6 (14)	C5—S4—C4—S3	-179.0 (4)
N4 ⁱⁱ —Cu1—N5—C6	126.4 (14)	C3—S3—C4—N3	6.7 (5)
N1 ⁱⁱⁱ —Cu1—N5—C6	37.7 (14)	C3—S3—C4—S4	-174.2 (3)
N1—Cu1—N5—C6	-142.3 (14)	N3—N4—C5—S4	0.8 (6)
N2—N1—C1—S1	0.3 (7)	Cu1 ^{iv} —N4—C5—S4	177.3 (3)
Cu1—N1—C1—S1	-172.5 (3)	C4—S4—C5—N4	-0.6 (5)

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

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C1—H1 \cdots O3 ^v	0.93	2.35	2.955 (8)	123
C3—H3A \cdots O1 ^{vi}	0.97	2.41	3.277 (9)	149
C5—H5 \cdots O1 ^{vii}	0.93	2.45	3.169 (9)	135

Symmetry codes: (v) $-x+1, -y+1, -z+1$; (vi) $-x+1/2, -y+3/2, -z+1$; (vii) $-x+1/2, y+1/2, -z+3/2$.