IUCrData

ISSN 2414-3146

catena-Poly[[[bis(acetonitrile-κN)(4,4′-dimethoxy-2,2′-bipyridine-$\kappa^2 N,N'$)copper(II)]-μ-trifluoromethanesulfonato-$\kappa^2 O:O'$] trifluoromethanesulfonate]

Rafael A. Adrian,[a]* Diego R. Hernandez[a] and Hadi D. Arman[b]

[a]Department of Chemistry and Biochemistry, University of the Incarnate Word, San Antonio, TX 78209, USA, and [b]Department of Chemistry, The University of Texas at San Antonio, San Antonio, TX 78249, USA. *Correspondence e-mail: adrian@uiwtx.edu

Received 22 September 2020
Accepted 21 October 2020

Edited by M. Weil, Vienna University of Technology, Austria

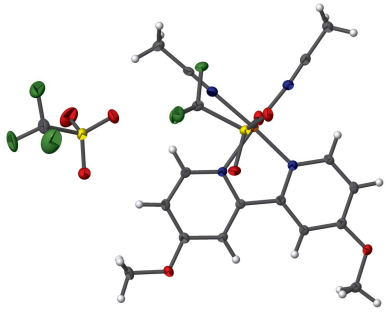
Keywords: crystal structure; copper(II); coordinating trifluoromethanesulfonate; trifluoromethanesulfonate salt; acetonitrile; 4,4′-dimethoxy-2,2′-bipyridine.

CCDC reference: 2039861

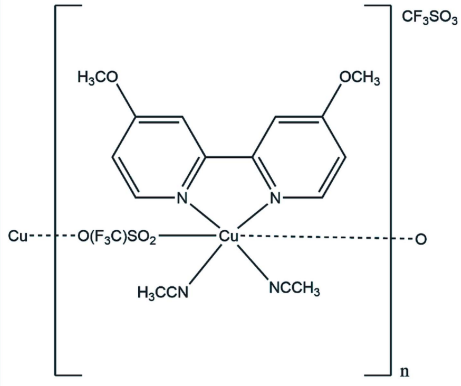
Structural data: full structural data are available from iucrdata.iucr.org

The central copper(II) atom of the title salt, $\{[Cu(CF_3SO_3)(CH_3CN)_2(C_{12}H_{12}N_2O_2)](CF_3SO_3)\}_n$ or $[[Cu(CH_3CN)_2(diOMe\text{-}bpy)(CF_3SO_3)](CF_3SO_3)]_n$ where diOMe-bpy is 4,4′-dimethoxy-2,2′-bipyridine, $C_{12}H_{12}N_2O_2$, is sixfold coordinated by the N atoms of the chelating bipyridine ligand, the N atoms of two acetonitrile molecules, and two trifluoromethanesulfonate O atoms in a tetragonally distorted octahedral shape. The formation of polymeric chains $[Cu(CH_3CN)_2(diOMe\text{-}bpy)(CF_3SO_3)]^+_n$ leaves voids for the non-coordinating trifluoromethanesulfonate anions that interact with the complex through weak hydrogen bonds. The presence of weakly coordinating ligands like acetonitrile and trifluoromethanesulfonate makes the title compound a convenient starting material for the synthesis of novel metal–organic frameworks.

3D view



Chemical scheme



Structure description

4,4′-Dimethoxy-2,2′-bipyridines are continuously being investigated for their photoluminescence features (Ravaro *et al.*, 2018), antimicrobial activity (Drzeżdżon *et al.*, 2019), good affinity in DNA binding (Anjomshoa *et al.*, 2016), and antitumor activity against human cancer cells (Qin *et al.*, 2019). As part of our research related to the coordination chemistry of metal ions with bipyridine and terpyridine ligands, in the present report we describe the synthesis and crystal structure of the title copper(II) complex salt, $[[Cu(CF_3SO_3)(C_2H_3N)_2(C_{12}H_{12}N_2O_2)](CF_3SO_3)]_n$.

As depicted in Fig. 1, the asymmetric unit of the title compound comprises a Cu^{II} atom, one *N*,*N*′-chelating 4,4′-dimethoxy-2,2′-bipyridine ligand, two acetonitrile ligands, and

Table 1
Selected geometric parameters (Å, °).

Cu1—O5^{i}	2.376 (2)	Cu1—N1	1.989 (2)
Cu1—O3	2.333 (2)	Cu1—N3	2.014 (2)
Cu1—N2	1.985 (2)	Cu1—N4	2.012 (2)
N2—Cu1—O5^{i}	90.71 (8)	N1—Cu1—N3	94.85 (10)
N2—Cu1—O3	94.76 (9)	N1—Cu1—N4	176.62 (9)
N2—Cu1—N1	81.56 (9)	N3—Cu1—O5^{i}	87.89 (9)
N2—Cu1—N3	175.99 (10)	N3—Cu1—O3	87.27 (9)
N2—Cu1—N4	95.12 (9)	N4—Cu1—O5^{i}	83.46 (9)
N1—Cu1—O5^{i}	95.88 (8)	N4—Cu1—O3	86.38 (9)
N1—Cu1—O3	94.53 (9)	N4—Cu1—N3	88.45 (10)

Symmetry code: (i) $x+1, y, z$.

two trifluoromethanesulfonate anions. The central copper(II) atom exhibits a tetragonally distorted octahedral coordination environment defined by the N atoms of the chelating 4,4′-dimethoxy-2,2′-bipyridine ligand and two neutral acetonitrile molecules in the equatorial plane and by two O atoms of symmetry-related trifluoromethanesulfonate anions in axial positions. Although the Cu—N bond lengths with the bipyridine ligand are shorter than the Cu—N bond lengths with the coordinating acetonitrile molecules, their values are comparable with the reported values of other copper(II) complexes with the same chelating ligand (Fettouhi, 2017). The acetonitrile ligands are bordering on linearity. All relevant bond lengths and angles involving the Cu^{II} atom are presented in Table 1. The cations in the title complex are aligned into polymeric chains extending parallel to the *a*-axis direction and pack into layers parallel to the *bc* plane, as illustrated in the crystal packing diagram given in Fig. 2. This arrangement leaves voids in which the second type of trifluoromethanesulfonate anions are located. These anions are non-coordinating and interact through hydrogen bonds.

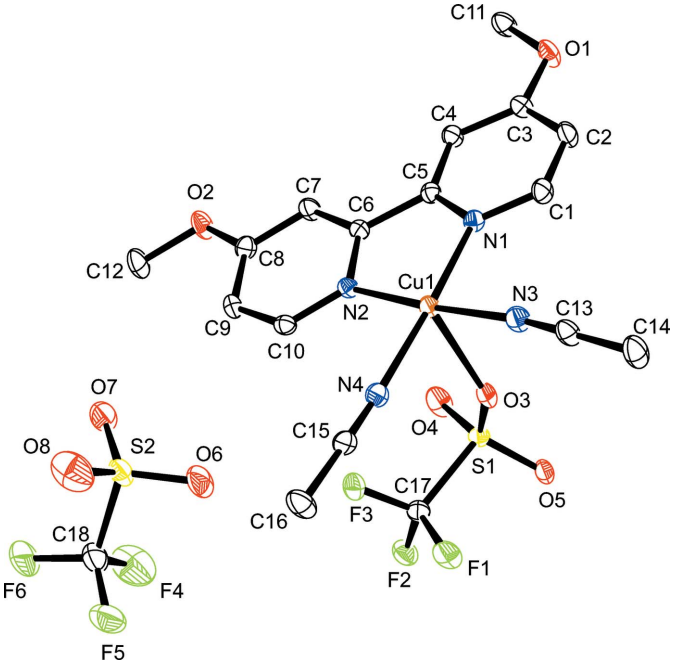


Figure 1
Asymmetric unit of the title compound with displacement ellipsoids drawn at the 50% probability level; H atoms are omitted for clarity.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O4^{ii}	0.95	2.23	3.175 (4)	177
C4—H4···O4^{ii}	0.95	2.37	3.315 (3)	175
C9—H9···O7	0.95	2.32	3.185 (4)	151
C16—H16*A*···O6	0.98	2.38	3.170 (4)	138
C14—H14*A*···O8^{iii}	0.98	2.35	3.194 (4)	144

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

Graph-set analysis is a method of analyzing hydrogen-bonding patterns in three-dimensional networks. Hydrogen-bonding patterns are classified into one of four pattern designators; rings (*R*), chains (*C*), intramolecular hydrogen-bonding patterns described as self (*S*), finite hydrogen-bonding patterns described as discrete (*D*). These designators include a superscript with the number of acceptor atoms, subscript with the number of donor atoms, and a number in parentheses indicating the number of atoms in the hydrogen-bonding motif (Grell *et al.*, 1999).

There are three types of hydrogen-bonding motifs present in the crystal lattice, with numerical values collated in Table 2. A centrosymmetric hydrogen-bonding ring, $R_2^1(7)$, occurs between the O4 atom on the coordinating trifluoromethanesulfonate anion with two hydrogen atoms on a 4,4′-dimethoxybipyridine molecule on a neighboring asymmetric unit. The non-coordinating trifluoromethanesulfonate anion forms a hydrogen-bonding ring, $R_2^2(12)$, through two C—H···O interactions with the O6 and O7 atoms. The other oxygen atom, O8, on the non-coordinating trifluoromethanesulfonate anion, has a discrete hydrogen-bonding interaction, $D_1^1(3)$, with a neighboring coordinating acetonitrile molecule.

Synthesis and crystallization

To synthesize the title compound, 4,4′-dimethoxy-2,2′-bipyridine (0.105 g, 0.486 mmol) was suspended in 40 ml of acetonitrile and stirred for 15 min. Solid $CuCl_2·2H_2O$ (0.083 g, 0.49 mmol) was added to the suspension and heated with stirring at 323 K for 1 h. AgOTf (0.250 g, 0.972 mmol) was added to the mixture and stirred without heating for 2 h. After

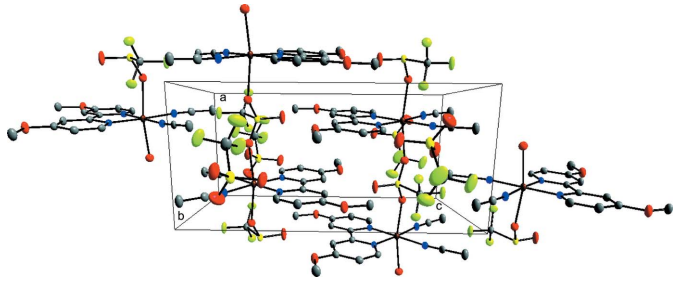


Figure 2
Perspective view of the packed structure of the title complex along the crystallographic *b* axis; H atoms are omitted for clarity.

the removal of AgCl by filtration, using a 0.45 μm PTFE syringe filter, the resulting blue solution was used to grow crystals by vapor diffusion with diethyl ether at 278 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The highest remaining electron density is located 0.93 Å from atom O3.

Acknowledgements

We are thankful for the support of the Department of Chemistry and Biochemistry at the University of the Incarnate Word and the X-ray Diffraction Laboratory at The University of Texas at San Antonio.

Funding information

Funding for this research was provided by: The Welch Foundation (award No. BN0032).

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cu(CF_3SO_3)(C_2H_3N)_2(C_{12}H_{12}N_2O_2)](CF_3O_3S)$
M_r	660.02
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	7.1004 (2), 12.0708 (4), 14.8155 (4)
α, β, γ (°)	87.368 (2), 89.436 (2), 76.819 (3)
V (Å^3)	1235.04 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.15
Crystal size (mm)	0.40 × 0.10 × 0.07
Data collection	
Diffractometer	XtaLAB AFC12 (RCD3): Kappa single
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2019)
T_{min}, T_{max}	0.884, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37314, 5666, 5392
R_{int}	0.040
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.125, 1.07
No. of reflections	5666
No. of parameters	356
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.01, −0.46

Computer programs: *CrysAlis PRO* (Rigaku OD, 2019), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

References

Anjomshoa, M., Torkzadeh-Mahani, M., Janczak, J., Rizzoli, C., Sahihi, M., Ataei, F. & Dehkhodaei, M. (2016). *Polyhedron*, **119**, 23–38.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Drzeżdżon, J., Piotrowska-Kirschling, A., Malinowski, J., Kloska, A., Gawdzik, B., Chmurzyński, L. & Jacewicz, D. (2019). *J. Mol. Liq.* **282**, 441–447.

Fettouhi, M. (2017). *Z. Kristallogr. New Cryst. Struct.* **232**, 985–986.

Grell, J., Bernstein, J. & Tinhofer, G. (1999). *Acta Cryst.* B**55**, 1030–1043.

Qin, Q. P., Wang, Z. F., Tan, M. X., Huang, X. L., Zou, H. H., Zou, B. Q., Shi, B. B. & Zhang, S. H. (2019). *Metallomics*, **11**, 1005–1015.

Ravaro, L. P., Mafud, A. C., Li, Z., Reinheimer, E., Simone, C. A., Mascarenhas, Y. P., Ford, P. C. & de Camargo, A. S. (2018). *Dyes Pigments*, **159**, 464–470.

Rigaku OD (2019). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2020). **5**, x201407 [https://doi.org/10.1107/S2414314620014078]

catena-Poly[[[bis(acetonitrile-κN)(4,4′-dimethoxy-2,2′-bipyridine-κ^2N,N')copper(II)]-μ-trifluoromethanesulfonato-$\kappa^2O:O'$] trifluoromethanesulfonate]

Rafael A. Adrian, Diego R. Hernandez and Hadi D. Arman

catena-Poly[[[bis(acetonitrile-κN)(4,4′-dimethoxy-2,2′-bipyridine-κ^2N,N')copper(II)]-μ-trifluoromethanesulfonato-$\kappa^2O:O'$] trifluoromethanesulfonate]

Crystal data

$[Cu(CF_3SO_3)(C_2H_3N)_2(C_{12}H_{12}N_2O_2)](CF_3O_3S)$
M_r = 660.02
Triclinic, $P\overline{1}$
a = 7.1004 (2) Å
b = 12.0708 (4) Å
c = 14.8155 (4) Å
α = 87.368 (2)°
β = 89.436 (2)°
γ = 76.819 (3)°
V = 1235.04 (6) Å^3
Z = 2
$F(000)$ = 666
D_x = 1.775 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 13491 reflections
θ = 2.7–29.0°
μ = 1.15 mm^{-1}
T = 100 K
Plate, clear light blue
0.40 × 0.10 × 0.07 mm

Data collection

XtaLAB AFC12 (RCD3): Kappa single diffractometer
Radiation source: Rotating-anode X-ray tube, Rigaku (Mo) X-ray Source
Mirror monochromator
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2019)
T_{min} = 0.884, T_{max} = 1.000
37314 measured reflections
5666 independent reflections
5392 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.5°, θ_{min} = 2.2°
h = −9→9
k = −15→15
l = −18→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.125
S = 1.07
5666 reflections
356 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 2.9P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.01 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.75757 (5)	0.42109 (3)	0.78071 (2)	0.01474 (11)
S1	0.23675 (10)	0.48568 (6)	0.76732 (4)	0.01596 (15)
S2	0.61504 (12)	0.95110 (6)	0.80753 (5)	0.02364 (18)
F3	0.3180 (3)	0.67475 (15)	0.81898 (12)	0.0238 (4)
F2	0.0138 (3)	0.67978 (15)	0.81561 (13)	0.0247 (4)
F1	0.1895 (3)	0.58506 (16)	0.92313 (12)	0.0299 (4)
O5	0.0885 (3)	0.42653 (17)	0.79453 (14)	0.0197 (4)
O3	0.4282 (3)	0.42680 (17)	0.79606 (15)	0.0215 (4)
O4	0.2216 (4)	0.53393 (19)	0.67652 (14)	0.0315 (6)
O2	0.6860 (3)	0.74737 (17)	0.44968 (14)	0.0244 (5)
O1	0.8576 (3)	0.12536 (17)	0.45169 (14)	0.0238 (5)
F5	0.3647 (4)	1.0672 (2)	0.91972 (16)	0.0500 (6)
N2	0.7231 (3)	0.53835 (19)	0.68011 (15)	0.0143 (4)
F6	0.4294 (4)	1.16541 (18)	0.80405 (19)	0.0536 (7)
N1	0.7950 (3)	0.3178 (2)	0.67802 (16)	0.0151 (4)
O6	0.5595 (4)	0.84920 (19)	0.84105 (17)	0.0369 (6)
O7	0.6329 (4)	0.9614 (2)	0.71066 (16)	0.0336 (6)
N3	0.8040 (4)	0.2945 (2)	0.87692 (16)	0.0198 (5)
F4	0.2473 (4)	1.0479 (2)	0.7904 (2)	0.0594 (7)
N4	0.7207 (4)	0.5332 (2)	0.87937 (16)	0.0176 (5)
C6	0.7481 (4)	0.4965 (2)	0.59648 (18)	0.0146 (5)
C5	0.7856 (4)	0.3705 (2)	0.59509 (18)	0.0147 (5)
O8	0.7668 (4)	0.9828 (3)	0.8563 (2)	0.0505 (8)
C7	0.7353 (4)	0.5661 (2)	0.51903 (19)	0.0177 (5)
H7	0.752622	0.534456	0.461161	0.021*
C15	0.7130 (4)	0.5956 (2)	0.93529 (18)	0.0175 (6)
C4	0.8068 (4)	0.3119 (2)	0.51601 (19)	0.0165 (5)
H4	0.801421	0.351339	0.458761	0.020*
C17	0.1866 (4)	0.6126 (2)	0.83457 (19)	0.0181 (5)
C9	0.6697 (4)	0.7277 (2)	0.61315 (19)	0.0172 (5)
H9	0.641922	0.807505	0.620840	0.021*
C8	0.6961 (4)	0.6845 (2)	0.52759 (19)	0.0176 (5)
C13	0.8214 (4)	0.2295 (2)	0.9359 (2)	0.0202 (6)
C10	0.6850 (4)	0.6514 (2)	0.68725 (19)	0.0161 (5)
H10	0.667564	0.680938	0.745858	0.019*
C3	0.8363 (4)	0.1932 (2)	0.52261 (19)	0.0181 (6)
C2	0.8441 (5)	0.1391 (2)	0.6079 (2)	0.0208 (6)
H2	0.863236	0.058601	0.614073	0.025*
C1	0.8236 (4)	0.2034 (2)	0.68297 (19)	0.0184 (6)

H1	0.829999	0.165612	0.740916	0.022*
C16	0.7075 (5)	0.6759 (3)	1.0062 (2)	0.0272 (7)
H16A	0.681353	0.753596	0.979411	0.041*
H16B	0.832382	0.659186	1.037540	0.041*
H16C	0.605032	0.668817	1.049419	0.041*
C14	0.8362 (5)	0.1454 (3)	1.0107 (2)	0.0274 (7)
H14A	0.822734	0.072737	0.987782	0.041*
H14B	0.733475	0.171786	1.054573	0.041*
H14C	0.962531	0.135124	1.040026	0.041*
C11	0.8548 (5)	0.1775 (3)	0.3622 (2)	0.0233 (6)
H11A	0.869985	0.118684	0.317564	0.035*
H11B	0.961202	0.216662	0.356008	0.035*
H11C	0.731362	0.232593	0.352245	0.035*
C18	0.4039 (5)	1.0638 (3)	0.8315 (2)	0.0309 (7)
C12	0.6424 (5)	0.8692 (2)	0.4558 (2)	0.0261 (7)
H12A	0.633264	0.905278	0.394865	0.039*
H12B	0.745317	0.891233	0.489377	0.039*
H12C	0.518965	0.894066	0.487237	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02004 (19)	0.01336 (18)	0.01075 (17)	−0.00366 (13)	−0.00062 (12)	−0.00033 (12)
S1	0.0205 (3)	0.0159 (3)	0.0118 (3)	−0.0046 (3)	0.0001 (2)	−0.0019 (2)
S2	0.0348 (4)	0.0170 (3)	0.0196 (4)	−0.0064 (3)	−0.0015 (3)	−0.0030 (3)
F3	0.0251 (9)	0.0198 (9)	0.0292 (10)	−0.0097 (7)	−0.0002 (7)	−0.0047 (7)
F2	0.0228 (9)	0.0184 (8)	0.0310 (10)	−0.0005 (7)	−0.0001 (7)	−0.0025 (7)
F1	0.0532 (13)	0.0235 (9)	0.0120 (8)	−0.0063 (9)	0.0011 (8)	−0.0025 (7)
O5	0.0225 (10)	0.0133 (9)	0.0237 (10)	−0.0048 (8)	−0.0003 (8)	−0.0009 (8)
O3	0.0226 (11)	0.0142 (10)	0.0278 (11)	−0.0039 (8)	0.0009 (9)	−0.0017 (8)
O4	0.0613 (17)	0.0207 (11)	0.0113 (10)	−0.0068 (11)	0.0002 (10)	−0.0001 (8)
O2	0.0413 (13)	0.0137 (10)	0.0174 (10)	−0.0048 (9)	−0.0019 (9)	0.0026 (8)
O1	0.0406 (13)	0.0139 (10)	0.0159 (10)	−0.0035 (9)	−0.0011 (9)	−0.0025 (8)
F5	0.0767 (18)	0.0344 (12)	0.0375 (13)	−0.0086 (12)	0.0220 (12)	−0.0112 (10)
N2	0.0167 (11)	0.0141 (11)	0.0123 (10)	−0.0037 (9)	−0.0011 (8)	−0.0015 (8)
F6	0.0781 (18)	0.0147 (10)	0.0640 (17)	−0.0041 (11)	0.0229 (14)	0.0023 (10)
N1	0.0169 (11)	0.0144 (11)	0.0141 (11)	−0.0037 (9)	−0.0006 (9)	−0.0008 (8)
O6	0.0630 (18)	0.0161 (11)	0.0296 (13)	−0.0063 (11)	0.0090 (12)	0.0034 (9)
O7	0.0578 (17)	0.0232 (12)	0.0214 (12)	−0.0130 (11)	0.0093 (11)	−0.0020 (9)
N3	0.0271 (13)	0.0184 (12)	0.0141 (11)	−0.0054 (10)	−0.0006 (10)	−0.0004 (9)
F4	0.0390 (14)	0.0580 (17)	0.077 (2)	0.0013 (12)	−0.0125 (13)	−0.0180 (14)
N4	0.0198 (12)	0.0176 (11)	0.0149 (11)	−0.0032 (9)	0.0004 (9)	0.0007 (9)
C6	0.0155 (12)	0.0150 (13)	0.0133 (12)	−0.0034 (10)	0.0004 (10)	−0.0015 (10)
C5	0.0144 (12)	0.0153 (13)	0.0146 (12)	−0.0039 (10)	−0.0011 (10)	0.0000 (10)
O8	0.0450 (17)	0.0538 (18)	0.0533 (18)	−0.0083 (14)	−0.0141 (14)	−0.0214 (15)
C7	0.0246 (14)	0.0161 (13)	0.0126 (12)	−0.0042 (11)	−0.0014 (10)	−0.0021 (10)
C15	0.0216 (14)	0.0168 (13)	0.0124 (12)	−0.0017 (11)	0.0003 (10)	0.0035 (10)
C4	0.0197 (13)	0.0137 (12)	0.0152 (13)	−0.0023 (10)	−0.0007 (10)	0.0004 (10)

C17	0.0218 (14)	0.0185 (13)	0.0145 (13)	−0.0050 (11)	0.0014 (10)	−0.0022 (10)
C9	0.0197 (13)	0.0122 (12)	0.0195 (14)	−0.0033 (10)	−0.0015 (11)	−0.0009 (10)
C8	0.0197 (13)	0.0167 (13)	0.0167 (13)	−0.0048 (11)	−0.0012 (10)	0.0010 (10)
C13	0.0248 (15)	0.0170 (13)	0.0189 (14)	−0.0042 (11)	−0.0025 (11)	−0.0036 (11)
C10	0.0173 (13)	0.0158 (13)	0.0152 (13)	−0.0035 (10)	0.0007 (10)	−0.0028 (10)
C3	0.0209 (14)	0.0157 (13)	0.0171 (13)	−0.0028 (11)	−0.0007 (11)	−0.0031 (10)
C2	0.0287 (15)	0.0118 (12)	0.0211 (14)	−0.0033 (11)	0.0001 (12)	−0.0003 (10)
C1	0.0241 (14)	0.0146 (13)	0.0156 (13)	−0.0033 (11)	−0.0006 (11)	0.0031 (10)
C16	0.0411 (19)	0.0219 (15)	0.0171 (14)	−0.0038 (13)	−0.0012 (13)	−0.0038 (12)
C14	0.045 (2)	0.0185 (14)	0.0191 (15)	−0.0086 (13)	−0.0028 (13)	0.0019 (11)
C11	0.0338 (17)	0.0190 (14)	0.0151 (14)	−0.0016 (12)	0.0001 (12)	−0.0023 (11)
C18	0.0414 (19)	0.0191 (15)	0.0317 (18)	−0.0058 (14)	0.0046 (15)	−0.0012 (13)
C12	0.0390 (18)	0.0121 (13)	0.0260 (16)	−0.0042 (12)	−0.0032 (13)	0.0031 (11)

Geometric parameters (Å, º)

Cu1—O5^{i}	2.376 (2)	C6—C5	1.484 (4)
Cu1—O3	2.333 (2)	C6—C7	1.382 (4)
Cu1—N2	1.985 (2)	C5—C4	1.386 (4)
Cu1—N1	1.989 (2)	C7—H7	0.9500
Cu1—N3	2.014 (2)	C7—C8	1.403 (4)
Cu1—N4	2.012 (2)	C15—C16	1.456 (4)
S1—O5	1.445 (2)	C4—H4	0.9500
S1—O3	1.442 (2)	C4—C3	1.399 (4)
S1—O4	1.436 (2)	C9—H9	0.9500
S1—C17	1.831 (3)	C9—C8	1.388 (4)
S2—O6	1.441 (2)	C9—C10	1.389 (4)
S2—O7	1.442 (2)	C13—C14	1.456 (4)
S2—O8	1.435 (3)	C10—H10	0.9500
S2—C18	1.824 (4)	C3—C2	1.391 (4)
F3—C17	1.336 (3)	C2—H2	0.9500
F2—C17	1.332 (3)	C2—C1	1.374 (4)
F1—C17	1.338 (3)	C1—H1	0.9500
O2—C8	1.345 (3)	C16—H16A	0.9800
O2—C12	1.439 (3)	C16—H16B	0.9800
O1—C3	1.348 (3)	C16—H16C	0.9800
O1—C11	1.439 (3)	C14—H14A	0.9800
F5—C18	1.335 (4)	C14—H14B	0.9800
N2—C6	1.354 (3)	C14—H14C	0.9800
N2—C10	1.339 (4)	C11—H11A	0.9800
F6—C18	1.325 (4)	C11—H11B	0.9800
N1—C5	1.353 (3)	C11—H11C	0.9800
N1—C1	1.348 (4)	C12—H12A	0.9800
N3—C13	1.136 (4)	C12—H12B	0.9800
F4—C18	1.328 (5)	C12—H12C	0.9800
N4—C15	1.138 (4)		
O3—Cu1—O5^{i}	168.85 (8)	F2—C17—S1	112.0 (2)

N2—Cu1—O5^{i}	90.71 (8)	F2—C17—F3	107.2 (2)
N2—Cu1—O3	94.76 (9)	F2—C17—F1	107.3 (2)
N2—Cu1—N1	81.56 (9)	F1—C17—S1	111.5 (2)
N2—Cu1—N3	175.99 (10)	C8—C9—H9	120.8
N2—Cu1—N4	95.12 (9)	C8—C9—C10	118.3 (3)
N1—Cu1—O5^{i}	95.88 (8)	C10—C9—H9	120.8
N1—Cu1—O3	94.53 (9)	O2—C8—C7	115.7 (3)
N1—Cu1—N3	94.85 (10)	O2—C8—C9	125.2 (3)
N1—Cu1—N4	176.62 (9)	C9—C8—C7	119.1 (3)
N3—Cu1—O5^{i}	87.89 (9)	N3—C13—C14	177.8 (3)
N3—Cu1—O3	87.27 (9)	N2—C10—C9	123.2 (3)
N4—Cu1—O5^{i}	83.46 (9)	N2—C10—H10	118.4
N4—Cu1—O3	86.38 (9)	C9—C10—H10	118.4
N4—Cu1—N3	88.45 (10)	O1—C3—C4	124.8 (3)
O5—S1—C17	104.08 (13)	O1—C3—C2	116.3 (3)
O3—S1—O5	113.46 (12)	C2—C3—C4	118.8 (3)
O3—S1—C17	103.30 (13)	C3—C2—H2	120.4
O4—S1—O5	115.66 (15)	C1—C2—C3	119.2 (3)
O4—S1—O3	115.70 (15)	C1—C2—H2	120.4
O4—S1—C17	102.27 (13)	N1—C1—C2	122.8 (3)
O6—S2—O7	114.84 (15)	N1—C1—H1	118.6
O6—S2—C18	103.34 (16)	C2—C1—H1	118.6
O7—S2—C18	103.15 (16)	C15—C16—H16A	109.5
O8—S2—O6	115.89 (19)	C15—C16—H16B	109.5
O8—S2—O7	114.17 (19)	C15—C16—H16C	109.5
O8—S2—C18	103.02 (18)	H16A—C16—H16B	109.5
S1—O5—Cu1^{ii}	145.62 (13)	H16A—C16—H16C	109.5
S1—O3—Cu1	144.69 (13)	H16B—C16—H16C	109.5
C8—O2—C12	117.2 (2)	C13—C14—H14A	109.5
C3—O1—C11	118.2 (2)	C13—C14—H14B	109.5
C6—N2—Cu1	114.82 (18)	C13—C14—H14C	109.5
C10—N2—Cu1	126.88 (19)	H14A—C14—H14B	109.5
C10—N2—C6	118.3 (2)	H14A—C14—H14C	109.5
C5—N1—Cu1	115.06 (18)	H14B—C14—H14C	109.5
C1—N1—Cu1	126.97 (19)	O1—C11—H11A	109.5
C1—N1—C5	117.9 (2)	O1—C11—H11B	109.5
C13—N3—Cu1	174.2 (2)	O1—C11—H11C	109.5
C15—N4—Cu1	175.4 (2)	H11A—C11—H11B	109.5
N2—C6—C5	114.5 (2)	H11A—C11—H11C	109.5
N2—C6—C7	122.4 (2)	H11B—C11—H11C	109.5
C7—C6—C5	123.1 (2)	F5—C18—S2	111.6 (2)
N1—C5—C6	114.0 (2)	F6—C18—S2	111.7 (3)
N1—C5—C4	122.8 (2)	F6—C18—F5	107.5 (3)
C4—C5—C6	123.2 (2)	F6—C18—F4	107.8 (3)
C6—C7—H7	120.7	F4—C18—S2	111.2 (2)
C6—C7—C8	118.6 (3)	F4—C18—F5	106.9 (3)
C8—C7—H7	120.7	O2—C12—H12A	109.5
N4—C15—C16	178.7 (3)	O2—C12—H12B	109.5

C5—C4—H4	120.8	O2—C12—H12C	109.5
C5—C4—C3	118.3 (3)	H12A—C12—H12B	109.5
C3—C4—H4	120.8	H12A—C12—H12C	109.5
F3—C17—S1	111.09 (19)	H12B—C12—H12C	109.5
F3—C17—F1	107.6 (2)		

Cu1—N2—C6—C5	3.3 (3)	O7—S2—C18—F4	60.7 (3)
Cu1—N2—C6—C7	−178.0 (2)	C6—N2—C10—C9	0.0 (4)
Cu1—N2—C10—C9	177.6 (2)	C6—C5—C4—C3	−178.2 (3)
Cu1—N1—C5—C6	−0.2 (3)	C6—C7—C8—O2	179.9 (3)
Cu1—N1—C5—C4	−179.5 (2)	C6—C7—C8—C9	−0.6 (4)
Cu1—N1—C1—C2	178.6 (2)	C5—N1—C1—C2	0.2 (4)
O5—S1—O3—Cu1	169.10 (19)	C5—C6—C7—C8	179.0 (3)
O5—S1—C17—F3	177.75 (19)	C5—C4—C3—O1	179.4 (3)
O5—S1—C17—F2	−62.4 (2)	C5—C4—C3—C2	−0.3 (4)
O5—S1—C17—F1	57.8 (2)	O8—S2—C18—F5	−61.0 (3)
O3—S1—O5—Cu1^{ii}	−171.80 (19)	O8—S2—C18—F6	59.4 (3)
O3—S1—C17—F3	59.0 (2)	O8—S2—C18—F4	179.7 (3)
O3—S1—C17—F2	178.83 (19)	C7—C6—C5—N1	179.3 (3)
O3—S1—C17—F1	−61.0 (2)	C7—C6—C5—C4	−1.5 (4)
O4—S1—O5—Cu1^{ii}	−34.7 (3)	C4—C3—C2—C1	−0.4 (4)
O4—S1—O3—Cu1	32.0 (3)	C17—S1—O5—Cu1^{ii}	76.6 (2)
O4—S1—C17—F3	−61.5 (2)	C17—S1—O3—Cu1	−78.9 (2)
O4—S1—C17—F2	58.3 (2)	C8—C9—C10—N2	−0.3 (4)
O4—S1—C17—F1	178.5 (2)	C10—N2—C6—C5	−178.8 (2)
O1—C3—C2—C1	179.9 (3)	C10—N2—C6—C7	−0.1 (4)
N2—C6—C5—N1	−2.0 (3)	C10—C9—C8—O2	−180.0 (3)
N2—C6—C5—C4	177.2 (3)	C10—C9—C8—C7	0.6 (4)
N2—C6—C7—C8	0.4 (4)	C3—C2—C1—N1	0.4 (5)
N1—C5—C4—C3	1.0 (4)	C1—N1—C5—C6	178.3 (2)
O6—S2—C18—F5	60.1 (3)	C1—N1—C5—C4	−0.9 (4)
O6—S2—C18—F6	−179.6 (3)	C11—O1—C3—C4	1.6 (4)
O6—S2—C18—F4	−59.2 (3)	C11—O1—C3—C2	−178.7 (3)
O7—S2—C18—F5	180.0 (3)	C12—O2—C8—C7	178.8 (3)
O7—S2—C18—F6	−59.7 (3)	C12—O2—C8—C9	−0.6 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O4^{iii}	0.95	2.23	3.175 (4)	177
C4—H4···O4^{iii}	0.95	2.37	3.315 (3)	175
C9—H9···O7	0.95	2.32	3.185 (4)	151
C16—H16*A*···O6	0.98	2.38	3.170 (4)	138
C14—H14*A*···O8^{iv}	0.98	2.35	3.194 (4)	144

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