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## Structure Reports

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# Poly[[ $(\mu_2$ -di-3-pyridylmethanone- $\kappa^2$ N:N')( $\mu_2$ -hexafluorosilicato- $\kappa^2$ F:F')-copper(II)] dihydrate]

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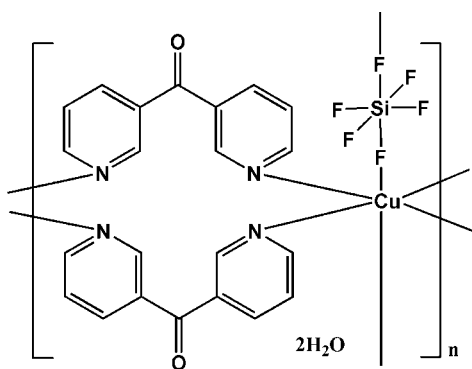
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 Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.094; data-to-parameter ratio = 12.0.

In the title complex,  $\{[\text{Cu}(\text{SiF}_6)(\text{C}_{11}\text{H}_8\text{N}_2\text{O}_2)] \cdot 2\text{H}_2\text{O}\}_n$ , the  $\text{Cu}^{\text{II}}$  atom adopts an  $\text{N}_4\text{F}_2$ -octahedral coordination geometry with four pyridine N atoms in the equatorial sites and two F atoms in the axial sites. The di-3-pyridylmethanone and hexafluorosilicate ligands act as bidentate ligands, linking symmetry-related  $\text{Cu}^{\text{II}}$  atoms. Water molecules form  $\text{O}-\text{H} \cdots \text{O}$  and  $\text{O}-\text{H} \cdots \text{F}$  hydrogen bonds with the di-3-pyridylmethanone and hexafluorosilicate ligands. The  $\text{Cu}^{2+}$  and  $\text{SiF}_6^{2-}$  ions are each located on a twofold axis.

## Related literature

For background to the coordination chemistry of pyridyl-based derivatives, see: Manriquez *et al.* (1991); Wang *et al.* (2009). For dipyridylmethanone, see: Boudalis *et al.* (2003). For transition metal complexes of di-3-pyridylmethanone, see: Chen *et al.* (2005, 2009); Chen & Mak (2005).



## Experimental

## Crystal data

 $[\text{Cu}(\text{SiF}_6)(\text{C}_{11}\text{H}_8\text{N}_2\text{O}_2)] \cdot 2\text{H}_2\text{O}$ 
 $M_r = 610.05$ 

 Monoclinic,  $C2/c$   
 $a = 22.276$  (3) Å  
 $b = 8.0625$  (11) Å  
 $c = 15.773$  (2) Å  
 $\beta = 123.757$  (2)°  
 $V = 2355.2$  (5) Å<sup>3</sup>
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.07$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.40 \times 0.32 \times 0.30$  mm

## Data collection

 Bruker SMART APEXII CCD  
 area-detector diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2007)  
 $T_{\text{min}} = 0.742$ ,  $T_{\text{max}} = 1.000$ 

 6195 measured reflections  
 2082 independent reflections  
 1822 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.094$   
 $S = 1.02$   
 2082 reflections

 174 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.54$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O1W}-\text{H1B} \cdots \text{F1}$	0.89	1.89	2.777 (6)	173
$\text{O1W}-\text{H1A} \cdots \text{O1}^{\dagger}$	0.89	2.03	2.850 (3)	153

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

Data collection: APEX2 (Bruker, 2007); cell refinement: APEX2 and SAINT (Bruker, 2007); data reduction: SAINT; 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 and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AA2040).

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## supporting information

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## Poly[[ $(\mu_2$ -di-3-pyridylmethanone- $\kappa^2$ N:N')( $\mu_2$ -hexafluorosilicato- $\kappa^2$ F:F')copper(II)] dihydrate]

Yong-Li Yang

### S1. Comment

Pyridyl-based building blocks are widely used in construction various supramolecules of transition metal complexes (Manriquez *et al.* 1991; Wang *et al.*, 2009). Among them, dipyridylmethanone derivatives are famous for their versatile linkage behavior in numbers of coordination supramolecular assemblies (Boudalis *et al.*, 2003). Di-3-pyridinylmethanone was provided to act as a flexible  $\mu^2$ -bridging mode in many coordination frameworks, such as one-dimensional helical and zigzag chains (Chen & Mak, 2005), two-dimensional nets (Chen *et al.*, 2005) as well as honeycomb-like three-dimensional frameworks (Chen *et al.*, 2009). Herein, we report a new structure derived from di-3-pyridinylmethanone, namely  $\{[\text{Cu}(\text{C}_{11}\text{H}_8\text{N}_2\text{O})_2\text{SiF}_6] \cdot 2\text{H}_2\text{O}\}_n$ .

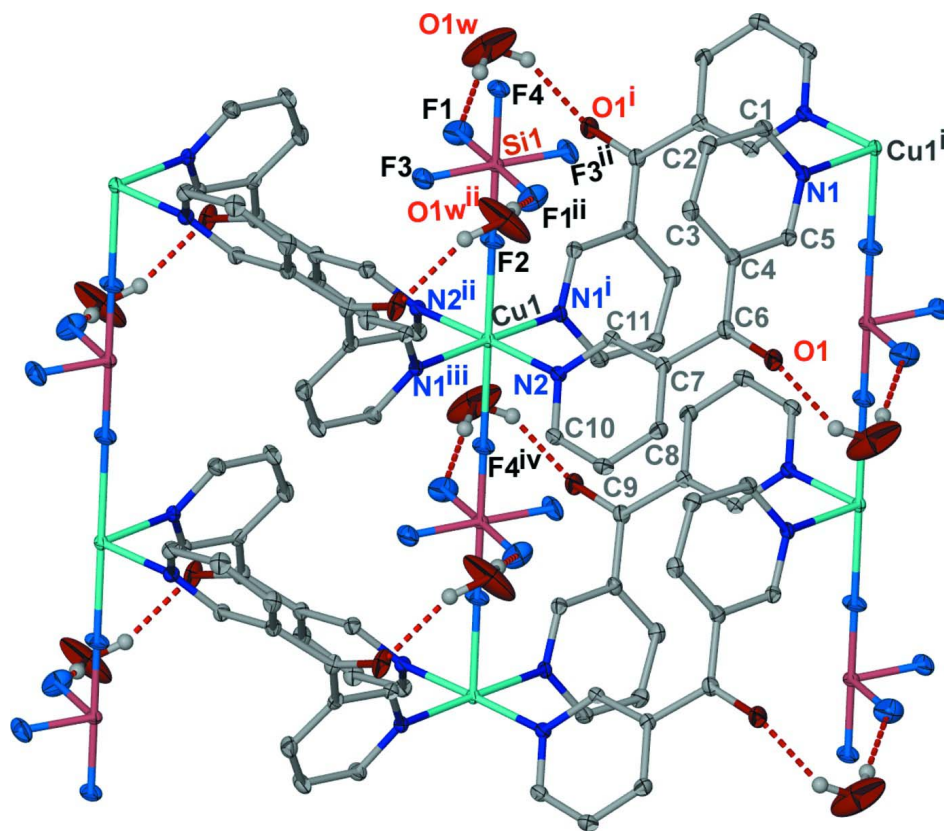
In the title complex, the  $\text{Cu}^{\text{II}}$  atom adopts an N4F2-octahedral coordination geometry with four pyridyl N atoms at the equatorial sites and two F atoms at the axial sites (Fig. 1). The di-3-pyridylmethanone and hexafluorosilicate ligands act as bidentate ligands linking symmetry-related  $\text{Cu}^{\text{II}}$  atoms. Water molecules form hydrogen bonds with di-3-pyridylmethanone and hexafluorosilicate ligands bridging them together (Table 1).  $\text{Cu}^{2+}$  and  $\text{SiF}_6^{2-}$  ions are located on a twofold axis, see Fig. 2 and Fig. 3. The structure of the title complex is remarkable different from a similar complex  $[(\text{Cu}L_2)(\text{BF}_4)_2]_n$  ( $L$  = di-3-pyridylmethanone, Chen *et al.* 2005), where the  $\text{Cu}^{\text{II}}$  adopts a square-plane N4-geometry with four ligands around the metal center, forming a (4,4) net structure.

### S2. Experimental

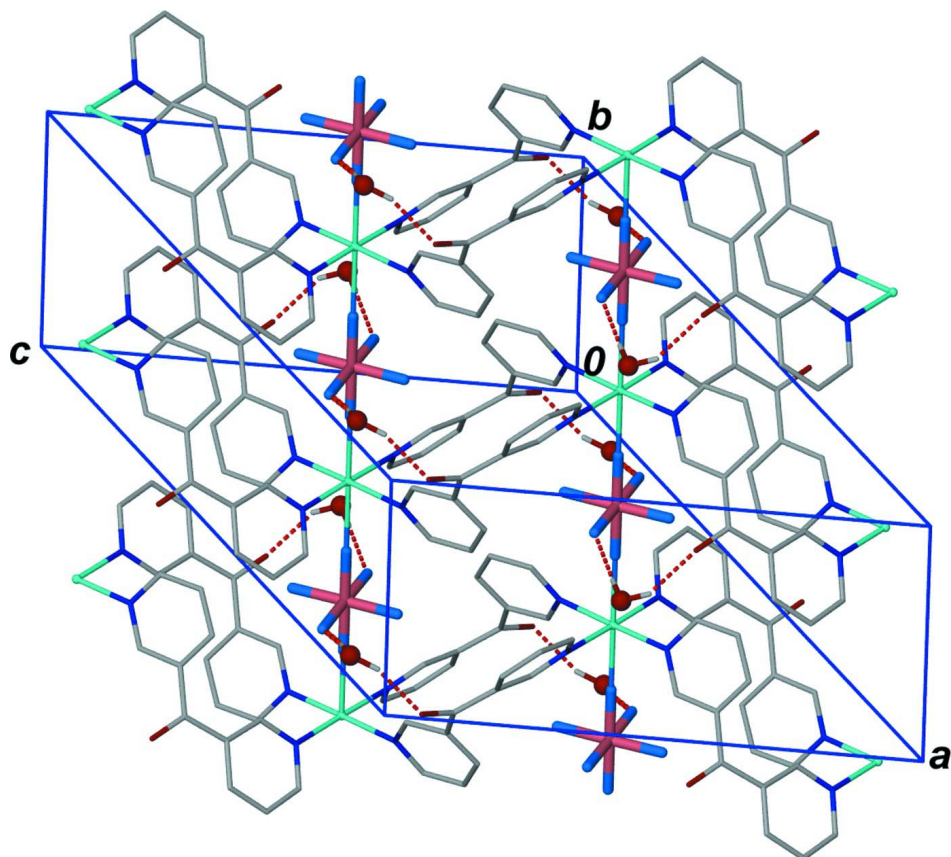
The ligand was obtained according to the reported procedure (Chen & Mak, 2005). The  $\text{Cu}(\text{BF}_4)_2 \cdot 6\text{H}_2\text{O}$  (35 mg, 0.1 mmol) and di-3-pyridylmethanone (38 mg, 0.2 mmol) were dissolved in a mixed solvent of 1 ml methanol and 3 ml acetonitrile with stirring at room temperature. The  $(\text{NH}_4)_2\text{SiF}_6$  (18 mg, 0.1 mmol) was subsequently added to the solution. After 4 hours, the resulted clear solution was filtered and the filtrate was left to stay in air. The block crystals suitable for x-ray diffraction analysis were obtained after about one week (29.9 mg, 49% yield).

### S3. Refinement

All the H atoms were located in the difference electron density maps but were placed in idealized positions and allowed to ride on the carrier atoms, with  $\text{C}-\text{H} = 0.93 \text{ \AA}$  and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

**Figure 1**

The title complex showing the atom-numbering scheme, with displacement ellipsoids shown at the 30% probability level. Hydrogen atoms are omitted for clarity. Symmetry codes: (i)  $-x+1, -y+1, -z+1$ ; (ii)  $-x+1, y, -z+0.5$ ; (iii)  $x, -y+1, z-0.5$ ; (iv)  $x, y+1, z$ .

**Figure 2**

Lateral view of the two-dimensional framework in the  $bc$  plane of the title complex. The O atoms of lattice water are shown as red ball mode. All H atoms except water H atoms are omitted for clarity. The Si—F are shown in a thick bond mode. The red dashed lines represent H-bonding interactions.

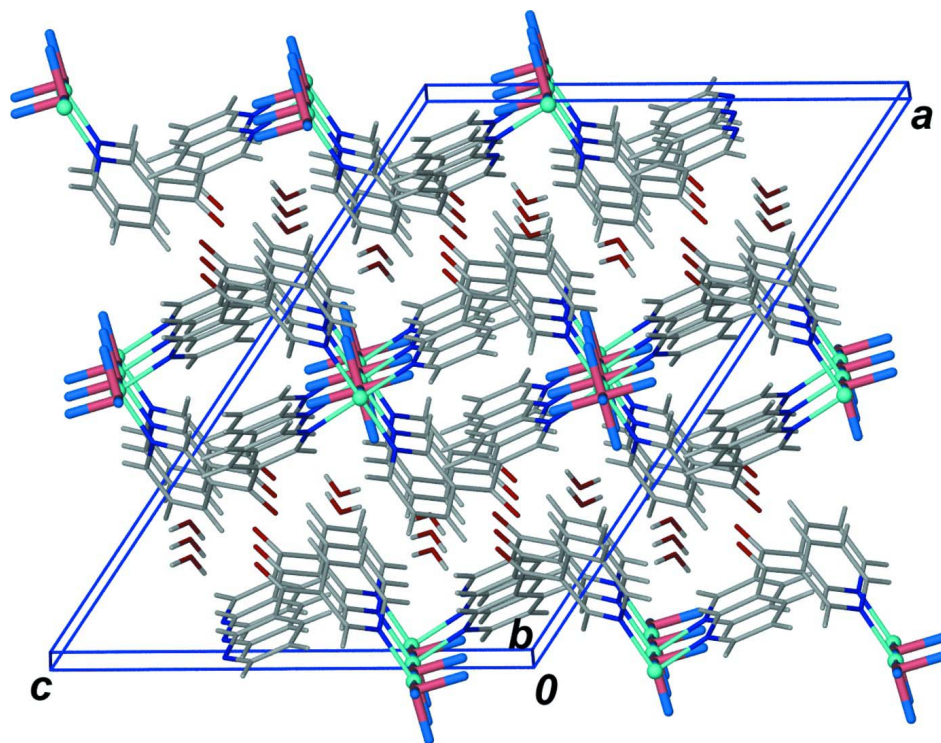


Figure 3

The packing diagram of the title complex.

**Poly[[ $(\mu_2$ -di-3-pyridylmethanone- $\kappa^2N:N')$ ]( $\mu_2$ - hexafluorosilicato- $\kappa^2F:F'$ )copper(II)] dihydrate]**

*Crystal data*

[Cu(SiF<sub>6</sub>)(C<sub>11</sub>H<sub>8</sub>N<sub>2</sub>O)<sub>2</sub>] $\cdot$ 2H<sub>2</sub>O

$M_r$  = 610.05

Monoclinic, *C2/c*

Hall symbol: -C 2yc

$a$  = 22.276 (3) Å

$b$  = 8.0625 (11) Å

$c$  = 15.773 (2) Å

$\beta$  = 123.757 (2)°

$V$  = 2355.2 (5) Å<sup>3</sup>

$Z$  = 4

$F(000)$  = 1236

$D_x$  = 1.720 Mg m<sup>-3</sup>

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

Cell parameters from 245 reflections

$\theta$  = 2.2–26.1°

$\mu$  = 1.07 mm<sup>-1</sup>

$T$  = 296 K

Block, blue

0.40 × 0.32 × 0.30 mm

*Data collection*

Bruker SMART APEXII CCD area-detector'  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2007)

$T_{\min}$  = 0.742,  $T_{\max}$  = 1.000

6195 measured reflections

2082 independent reflections

1822 reflections with  $I > 2\sigma(I)$

$R_{\text{int}}$  = 0.031

$\theta_{\text{max}}$  = 25.0°,  $\theta_{\text{min}}$  = 2.2°

$h$  = -22→26

$k$  = -8→9

$l$  = -18→16

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.094$	$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 3.641P]$ $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\max} < 0.001$
2082 reflections	$\Delta\rho_{\max} = 0.54 \text{ e } \text{Å}^{-3}$
174 parameters	$\Delta\rho_{\min} = -0.31 \text{ e } \text{Å}^{-3}$
0 restraints	
Primary atom site location: structure-invariant direct methods	

Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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  $F^2 > 2\sigma(F^2)$  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 ( $\text{Å}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.5000	0.74249 (4)	0.2500	0.02213 (16)
F1	0.41305 (11)	0.2547 (2)	0.15265 (16)	0.0656 (6)
F2	0.5000	0.4646 (2)	0.2500	0.0430 (6)
F3	0.52519 (13)	0.25362 (17)	0.16853 (16)	0.0567 (6)
F4	0.5000	0.0403 (2)	0.2500	0.0423 (5)
O1	0.71275 (11)	0.6013 (2)	0.74098 (13)	0.0495 (5)
N1	0.55932 (11)	0.2545 (2)	0.68811 (15)	0.0247 (4)
N2	0.59150 (11)	0.7466 (2)	0.39361 (16)	0.0255 (4)
C1	0.55661 (14)	0.1248 (3)	0.63175 (18)	0.0317 (5)
H1	0.5344	0.0272	0.6319	0.038*
C2	0.58540 (15)	0.1321 (3)	0.5744 (2)	0.0379 (6)
H2	0.5820	0.0409	0.5359	0.045*
C3	0.61944 (15)	0.2748 (3)	0.5736 (2)	0.0357 (6)
H3	0.6373	0.2834	0.5326	0.043*
C4	0.62620 (12)	0.4052 (3)	0.63604 (16)	0.0267 (5)
C5	0.59552 (12)	0.3905 (3)	0.69197 (17)	0.0260 (5)
H5	0.6002	0.4781	0.7336	0.031*
C7	0.66029 (13)	0.6594 (3)	0.56799 (17)	0.0271 (5)
C8	0.70977 (14)	0.7864 (3)	0.59181 (19)	0.0337 (6)
H8	0.7493	0.8005	0.6585	0.040*
C9	0.69953 (14)	0.8907 (3)	0.51563 (19)	0.0369 (6)
H9	0.7322	0.9753	0.5299	0.044*
C10	0.63992 (13)	0.8673 (3)	0.41792 (18)	0.0309 (5)
H10	0.6330	0.9382	0.3667	0.037*
C11	0.60197 (13)	0.6426 (3)	0.46786 (17)	0.0270 (5)

H11	0.5691	0.5573	0.4513	0.032*
C6	0.66989 (13)	0.5574 (3)	0.65383 (17)	0.0310 (5)
Si1	0.5000	0.25199 (9)	0.2500	0.0252 (2)
O1W	0.2808 (2)	0.1657 (6)	0.1183 (4)	0.168 (2)
H1A	0.2777	0.2089	0.1676	0.252*
H1B	0.3244	0.1856	0.1308	0.252*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.0264 (2)	0.0224 (2)	0.0210 (2)	0.000	0.01529 (19)	0.000
F1	0.0410 (11)	0.0637 (13)	0.0584 (13)	-0.0046 (8)	0.0067 (10)	0.0081 (8)
F2	0.0645 (15)	0.0182 (9)	0.0684 (15)	0.000	0.0506 (13)	0.000
F3	0.1013 (17)	0.0365 (9)	0.0722 (13)	-0.0090 (8)	0.0731 (13)	-0.0082 (7)
F4	0.0658 (15)	0.0203 (9)	0.0571 (14)	0.000	0.0442 (13)	0.000
O1	0.0502 (12)	0.0604 (13)	0.0247 (10)	-0.0200 (10)	0.0126 (9)	-0.0002 (8)
N1	0.0289 (11)	0.0259 (10)	0.0233 (10)	0.0010 (7)	0.0171 (9)	0.0014 (7)
N2	0.0282 (11)	0.0240 (10)	0.0259 (10)	-0.0003 (7)	0.0160 (9)	0.0008 (7)
C1	0.0396 (14)	0.0261 (12)	0.0355 (13)	-0.0020 (10)	0.0247 (11)	-0.0023 (10)
C2	0.0507 (16)	0.0341 (13)	0.0412 (14)	-0.0035 (11)	0.0332 (13)	-0.0097 (11)
C3	0.0418 (15)	0.0406 (14)	0.0334 (14)	-0.0016 (11)	0.0264 (12)	-0.0009 (11)
C4	0.0251 (12)	0.0301 (12)	0.0221 (11)	0.0032 (9)	0.0114 (10)	0.0056 (9)
C5	0.0276 (12)	0.0264 (11)	0.0235 (11)	0.0023 (9)	0.0139 (10)	0.0010 (9)
C7	0.0287 (12)	0.0284 (11)	0.0267 (11)	-0.0012 (9)	0.0170 (10)	0.0005 (9)
C8	0.0305 (13)	0.0378 (13)	0.0284 (13)	-0.0090 (11)	0.0136 (11)	-0.0047 (10)
C9	0.0386 (14)	0.0338 (13)	0.0400 (14)	-0.0112 (11)	0.0229 (12)	-0.0023 (11)
C10	0.0372 (13)	0.0271 (11)	0.0339 (12)	-0.0031 (10)	0.0232 (11)	0.0017 (10)
C11	0.0296 (12)	0.0256 (11)	0.0278 (12)	-0.0027 (9)	0.0172 (10)	0.0010 (9)
C6	0.0284 (12)	0.0372 (13)	0.0267 (12)	-0.0014 (10)	0.0149 (11)	0.0021 (10)
Si1	0.0328 (5)	0.0179 (5)	0.0280 (5)	0.000	0.0188 (4)	0.000
O1W	0.105 (3)	0.176 (4)	0.257 (5)	-0.047 (3)	0.121 (4)	-0.145 (4)

*Geometric parameters (Å, °)*

Cu1—N1 <sup>i</sup>	2.033 (2)	C2—H2	0.9300
Cu1—N1 <sup>ii</sup>	2.033 (2)	C3—C4	1.390 (3)
Cu1—N2	2.038 (2)	C3—H3	0.9300
Cu1—N2 <sup>iii</sup>	2.038 (2)	C4—C5	1.389 (3)
Cu1—F2	2.241 (2)	C4—C6	1.493 (3)
Cu1—F4 <sup>iv</sup>	2.401 (2)	C5—H5	0.9300
F1—Si1	1.6747 (19)	C7—C11	1.386 (3)
F2—Si1	1.714 (2)	C7—C8	1.394 (3)
F3—Si1	1.6636 (17)	C7—C6	1.494 (3)
F4—Si1	1.707 (2)	C8—C9	1.378 (4)
F4—Cu1 <sup>v</sup>	2.401 (2)	C8—H8	0.9300
O1—C6	1.212 (3)	C9—C10	1.378 (4)
N1—C5	1.342 (3)	C9—H9	0.9300
N1—C1	1.352 (3)	C10—H10	0.9300

N1—Cu1 <sup>ii</sup>	2.033 (2)	C11—H11	0.9300
N2—C10	1.341 (3)	Si1—F3 <sup>iii</sup>	1.6636 (17)
N2—C11	1.351 (3)	Si1—F1 <sup>iii</sup>	1.6747 (19)
C1—C2	1.371 (4)	O1W—H1A	0.8900
C1—H1	0.9300	O1W—H1B	0.8901
C2—C3	1.382 (4)		
N1 <sup>i</sup> —Cu1—N1 <sup>ii</sup>	178.65 (9)	N1—C5—H5	118.8
N1 <sup>i</sup> —Cu1—N2	91.03 (8)	C4—C5—H5	118.8
N1 <sup>ii</sup> —Cu1—N2	88.95 (8)	C11—C7—C8	118.6 (2)
N1 <sup>i</sup> —Cu1—N2 <sup>iii</sup>	88.95 (8)	C11—C7—C6	123.4 (2)
N1 <sup>ii</sup> —Cu1—N2 <sup>iii</sup>	91.03 (8)	C8—C7—C6	117.8 (2)
N2—Cu1—N2 <sup>iii</sup>	178.15 (9)	C9—C8—C7	119.4 (2)
N1 <sup>i</sup> —Cu1—F2	90.68 (5)	C9—C8—H8	120.3
N1 <sup>ii</sup> —Cu1—F2	90.68 (5)	C7—C8—H8	120.3
N2—Cu1—F2	90.93 (5)	C8—C9—C10	118.8 (2)
N2 <sup>iii</sup> —Cu1—F2	90.93 (5)	C8—C9—H9	120.6
N1 <sup>i</sup> —Cu1—F4 <sup>iv</sup>	89.32 (5)	C10—C9—H9	120.6
N1 <sup>ii</sup> —Cu1—F4 <sup>iv</sup>	89.32 (5)	N2—C10—C9	122.8 (2)
N2—Cu1—F4 <sup>iv</sup>	89.07 (5)	N2—C10—H10	118.6
N2 <sup>iii</sup> —Cu1—F4 <sup>iv</sup>	89.07 (5)	C9—C10—H10	118.6
F2—Cu1—F4 <sup>iv</sup>	180.0	N2—C11—C7	121.9 (2)
Si1—F2—Cu1	180.000 (1)	N2—C11—H11	119.1
Si1—F4—Cu1 <sup>v</sup>	180.000 (1)	C7—C11—H11	119.1
C5—N1—C1	117.9 (2)	O1—C6—C4	118.3 (2)
C5—N1—Cu1 <sup>ii</sup>	120.21 (15)	O1—C6—C7	119.5 (2)
C1—N1—Cu1 <sup>ii</sup>	121.42 (16)	C4—C6—C7	122.1 (2)
C10—N2—C11	118.6 (2)	F3—Si1—F3 <sup>iii</sup>	179.09 (11)
C10—N2—Cu1	118.57 (16)	F3—Si1—F1 <sup>iii</sup>	89.62 (12)
C11—N2—Cu1	122.52 (15)	F3 <sup>iii</sup> —Si1—F1 <sup>iii</sup>	90.36 (12)
N1—C1—C2	122.3 (2)	F3—Si1—F1	90.36 (12)
N1—C1—H1	118.8	F3 <sup>iii</sup> —Si1—F1	89.62 (12)
C2—C1—H1	118.8	F1 <sup>iii</sup> —Si1—F1	178.52 (13)
C1—C2—C3	120.2 (2)	F3—Si1—F4	90.45 (5)
C1—C2—H2	119.9	F3 <sup>iii</sup> —Si1—F4	90.45 (5)
C3—C2—H2	119.9	F1 <sup>iii</sup> —Si1—F4	90.74 (6)
C2—C3—C4	117.8 (2)	F1—Si1—F4	90.74 (6)
C2—C3—H3	121.1	F3—Si1—F2	89.55 (5)
C4—C3—H3	121.1	F3 <sup>iii</sup> —Si1—F2	89.55 (5)
C5—C4—C3	119.2 (2)	F1 <sup>iii</sup> —Si1—F2	89.26 (6)
C5—C4—C6	116.8 (2)	F1—Si1—F2	89.26 (6)
C3—C4—C6	123.9 (2)	F4—Si1—F2	180.0
N1—C5—C4	122.4 (2)	H1A—O1W—H1B	109.8
N1 <sup>i</sup> —Cu1—N2—C10	54.16 (18)	C11—C7—C8—C9	-0.2 (4)
N1 <sup>ii</sup> —Cu1—N2—C10	-124.49 (18)	C6—C7—C8—C9	-175.2 (2)
F2—Cu1—N2—C10	144.85 (17)	C7—C8—C9—C10	0.7 (4)
F4 <sup>iv</sup> —Cu1—N2—C10	-35.15 (17)	C11—N2—C10—C9	-0.6 (4)



N1 <sup>i</sup> —Cu1—N2—C11	-132.42 (18)	Cu1—N2—C10—C9	173.0 (2)
N1 <sup>ii</sup> —Cu1—N2—C11	48.93 (18)	C8—C9—C10—N2	-0.3 (4)
F2—Cu1—N2—C11	-41.73 (17)	C10—N2—C11—C7	1.2 (3)
F4 <sup>iv</sup> —Cu1—N2—C11	138.27 (17)	Cu1—N2—C11—C7	-172.22 (17)
C5—N1—C1—C2	-4.1 (4)	C8—C7—C11—N2	-0.8 (4)
Cu1 <sup>ii</sup> —N1—C1—C2	167.9 (2)	C6—C7—C11—N2	173.9 (2)
N1—C1—C2—C3	0.8 (4)	C5—C4—C6—O1	45.3 (3)
C1—C2—C3—C4	3.0 (4)	C3—C4—C6—O1	-129.8 (3)
C2—C3—C4—C5	-3.4 (4)	C5—C4—C6—C7	-132.4 (2)
C2—C3—C4—C6	171.6 (2)	C3—C4—C6—C7	52.6 (3)
C1—N1—C5—C4	3.7 (3)	C11—C7—C6—O1	-164.2 (2)
Cu1 <sup>ii</sup> —N1—C5—C4	-168.43 (17)	C8—C7—C6—O1	10.6 (4)
C3—C4—C5—N1	0.0 (3)	C11—C7—C6—C4	13.4 (4)
C6—C4—C5—N1	-175.3 (2)	C8—C7—C6—C4	-171.8 (2)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1 $W$ —H1 $B$ —F1	0.89	1.89	2.777 (6)	173
O1 $W$ —H1 $A$ —O1 <sup>ii</sup>	0.89	2.03	2.850 (3)	153

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