

Poly[[(μ_2 -di-3-pyridylmethanone- $\kappa^2 N:N'$)(μ_2 -hexafluorosilicato- $\kappa^2 F:F'$)-copper(II)] dihydrate]

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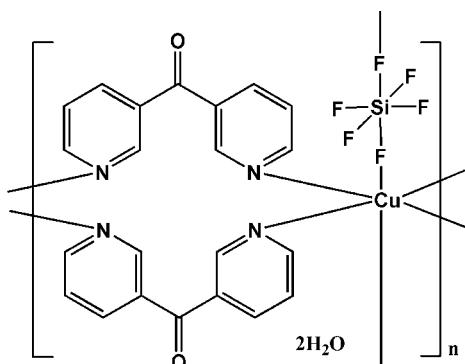
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(C-C) = 0.004$ Å;
 R factor = 0.034; wR factor = 0.094; data-to-parameter ratio = 12.0.

In the title complex, $\{[Cu(SiF_6)(C_{11}H_8N_2O)_2] \cdot 2H_2O\}_n$, the Cu^{II} atom adopts an N_4F_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 Cu^{II} atoms. Water molecules form O—H···O and O—H···F hydrogen bonds with the di-3-pyridylmethanone and hexafluorosilicate ligands. The Cu²⁺ and SiF₆²⁻ 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

[Cu(SiF₆)(C₁₁H₈N₂O)₂] · 2H₂O

$M_r = 610.05$

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) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.07$ mm⁻¹
 $T = 296$ 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)
 $T_{min} = 0.742$, $T_{max} = 1.000$

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

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⁻³
 $\Delta\rho_{\text{min}} = -0.31$ 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—H1B···F1	0.89	1.89	2.777 (6)	173
O1W—H1A···O1 ⁱ	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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supplementary materials

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Poly[[(μ_2 -di-3-pyridylmethanone- κ^2 N:N')(μ_2 -hexafluorosilicato- κ^2 F:F')copper(II)] dihydrate]

Y.-L. Yang

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 derivates 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 μ^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 Cu^{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 Cu^{II} atoms. Water molecules form hydrogen bonds with di-3-pyridylmethanone and hexafluorosilicate ligands bridging them together (Table 1). Cu²⁺ and SiF₆²⁻ 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 Cu^{II} adopts a square-plane N4-geometry with four ligands around the metal center, forming a (4,4) net structure.

Experimental

The ligand was obtained according to the reported procedure (Chen & Mak, 2005). The Cu(BF₄)₂·6H₂O (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 (NH₄)₂SiF₆ (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).

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 C—H = 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

supplementary materials

Figures

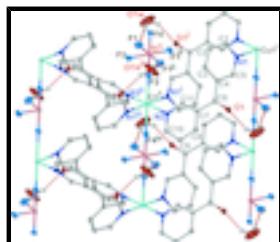


Fig. 1. The title complex showing the atom-numbering scheme, with displacement ellipsoids shown at the 30% probability level. Hydrogen atoms are omitted for clarity. Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, y, -z+0.5$; (iii) $x, -y+1, z-0.5$; (iv) $x, y+1, z$.

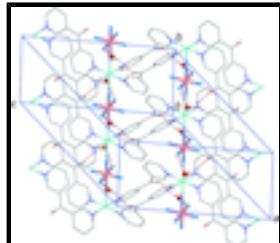


Fig. 2. Lateral view of the two-dimensional framework in the bc plane of the title complex. The O atoms of lattice water are shown as red ball mode. All H atoms except water H atoms are omitted for clarity. The Si—F are shown in a thick bond mode. The red dashed lines represent H-bonding interactions.

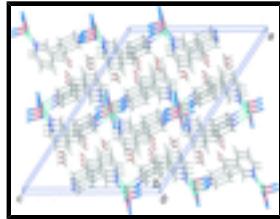


Fig. 3. The packing diagram of the title complex.

Poly[[(μ_2 -di-3-pyridylmethanone- $\kappa^2 N:N'$)(μ_2 - hexafluorosilicato- $\kappa^2 F:F'$)copper(II)] dihydrate]

Crystal data

$[Cu(SiF_6)(C_{11}H_8N_2O)_2] \cdot 2H_2O$	$F(000) = 1236$
$M_r = 610.05$	$D_x = 1.720 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -C 2yc	Cell parameters from 245 reflections
$a = 22.276 (3) \text{ \AA}$	$\theta = 2.2\text{--}26.1^\circ$
$b = 8.0625 (11) \text{ \AA}$	$\mu = 1.07 \text{ mm}^{-1}$
$c = 15.773 (2) \text{ \AA}$	$T = 296 \text{ K}$
$\beta = 123.757 (2)^\circ$	Block, blue
$V = 2355.2 (5) \text{ \AA}^3$	$0.40 \times 0.32 \times 0.30 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART APEXII CCD area-detector [†] diffractometer	2082 independent reflections
Radiation source: fine-focus sealed tube	1822 reflections with $I > 2\sigma(I)$
graphite	$R_{\text{int}} = 0.031$
ω scans	$\theta_{\text{max}} = 25.0^\circ, \theta_{\text{min}} = 2.2^\circ$
Absorption correction: multi-scan	$h = -22 \rightarrow 26$

(SADABS; Bruker, 2007)

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

6195 measured reflections

$k = -8 \rightarrow 9$

$l = -18 \rightarrow 16$

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full

Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.034$

Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.094$

H-atom parameters constrained

$S = 1.02$

$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 3.641P]$ $P = (F_o^2 + 2F_c^2)/3$

2082 reflections

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

174 parameters

$\Delta\rho_{\max} = 0.54 \text{ e \AA}^{-3}$

0 restraints

$\Delta\rho_{\min} = -0.31 \text{ e \AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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)

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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 (\AA^2)

	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 (\AA , $^\circ$)

Cu1—N1 ⁱ	2.033 (2)	C2—H2	0.9300
Cu1—N1 ⁱⁱ	2.033 (2)	C3—C4	1.390 (3)
Cu1—N2	2.038 (2)	C3—H3	0.9300
Cu1—N2 ⁱⁱⁱ	2.038 (2)	C4—C5	1.389 (3)

Cu1—F2	2.241 (2)	C4—C6	1.493 (3)
Cu1—F4 ^{iv}	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 ^v	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 ⁱⁱ	2.033 (2)	C11—H11	0.9300
N2—C10	1.341 (3)	Si1—F3 ⁱⁱⁱ	1.6636 (17)
N2—C11	1.351 (3)	Si1—F1 ⁱⁱⁱ	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 ⁱ —Cu1—N1 ⁱⁱ	178.65 (9)	N1—C5—H5	118.8
N1 ⁱ —Cu1—N2	91.03 (8)	C4—C5—H5	118.8
N1 ⁱⁱ —Cu1—N2	88.95 (8)	C11—C7—C8	118.6 (2)
N1 ⁱ —Cu1—N2 ⁱⁱⁱ	88.95 (8)	C11—C7—C6	123.4 (2)
N1 ⁱⁱ —Cu1—N2 ⁱⁱⁱ	91.03 (8)	C8—C7—C6	117.8 (2)
N2—Cu1—N2 ⁱⁱⁱ	178.15 (9)	C9—C8—C7	119.4 (2)
N1 ⁱ —Cu1—F2	90.68 (5)	C9—C8—H8	120.3
N1 ⁱⁱ —Cu1—F2	90.68 (5)	C7—C8—H8	120.3
N2—Cu1—F2	90.93 (5)	C8—C9—C10	118.8 (2)
N2 ⁱⁱⁱ —Cu1—F2	90.93 (5)	C8—C9—H9	120.6
N1 ⁱ —Cu1—F4 ^{iv}	89.32 (5)	C10—C9—H9	120.6
N1 ⁱⁱ —Cu1—F4 ^{iv}	89.32 (5)	N2—C10—C9	122.8 (2)
N2—Cu1—F4 ^{iv}	89.07 (5)	N2—C10—H10	118.6
N2 ⁱⁱⁱ —Cu1—F4 ^{iv}	89.07 (5)	C9—C10—H10	118.6
F2—Cu1—F4 ^{iv}	180.0	N2—C11—C7	121.9 (2)
Si1—F2—Cu1	180.000 (1)	N2—C11—H11	119.1
Si1—F4—Cu1 ^v	180.000 (1)	C7—C11—H11	119.1
C5—N1—C1	117.9 (2)	O1—C6—C4	118.3 (2)
C5—N1—Cu1 ⁱⁱ	120.21 (15)	O1—C6—C7	119.5 (2)
C1—N1—Cu1 ⁱⁱ	121.42 (16)	C4—C6—C7	122.1 (2)
C10—N2—C11	118.6 (2)	F3—Si1—F3 ⁱⁱⁱ	179.09 (11)
C10—N2—Cu1	118.57 (16)	F3—Si1—F1 ⁱⁱⁱ	89.62 (12)
C11—N2—Cu1	122.52 (15)	F3 ⁱⁱⁱ —Si1—F1 ⁱⁱⁱ	90.36 (12)
N1—C1—C2	122.3 (2)	F3—Si1—F1	90.36 (12)
N1—C1—H1	118.8	F3 ⁱⁱⁱ —Si1—F1	89.62 (12)
C2—C1—H1	118.8	F1 ⁱⁱⁱ —Si1—F1	178.52 (13)
C1—C2—C3	120.2 (2)	F3—Si1—F4	90.45 (5)

supplementary materials

C1—C2—H2	119.9	F3 ⁱⁱⁱ —Si1—F4	90.45 (5)
C3—C2—H2	119.9	F1 ⁱⁱⁱ —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 ⁱⁱⁱ —Si1—F2	89.55 (5)
C5—C4—C3	119.2 (2)	F1 ⁱⁱⁱ —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 ⁱ —Cu1—N2—C10	54.16 (18)	C11—C7—C8—C9	-0.2 (4)
N1 ⁱⁱ —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 ^{iv} —Cu1—N2—C10	-35.15 (17)	C11—N2—C10—C9	-0.6 (4)
N1 ⁱ —Cu1—N2—C11	-132.42 (18)	Cu1—N2—C10—C9	173.0 (2)
N1 ⁱⁱ —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 ^{iv} —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 ⁱⁱ —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 ⁱⁱ —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)

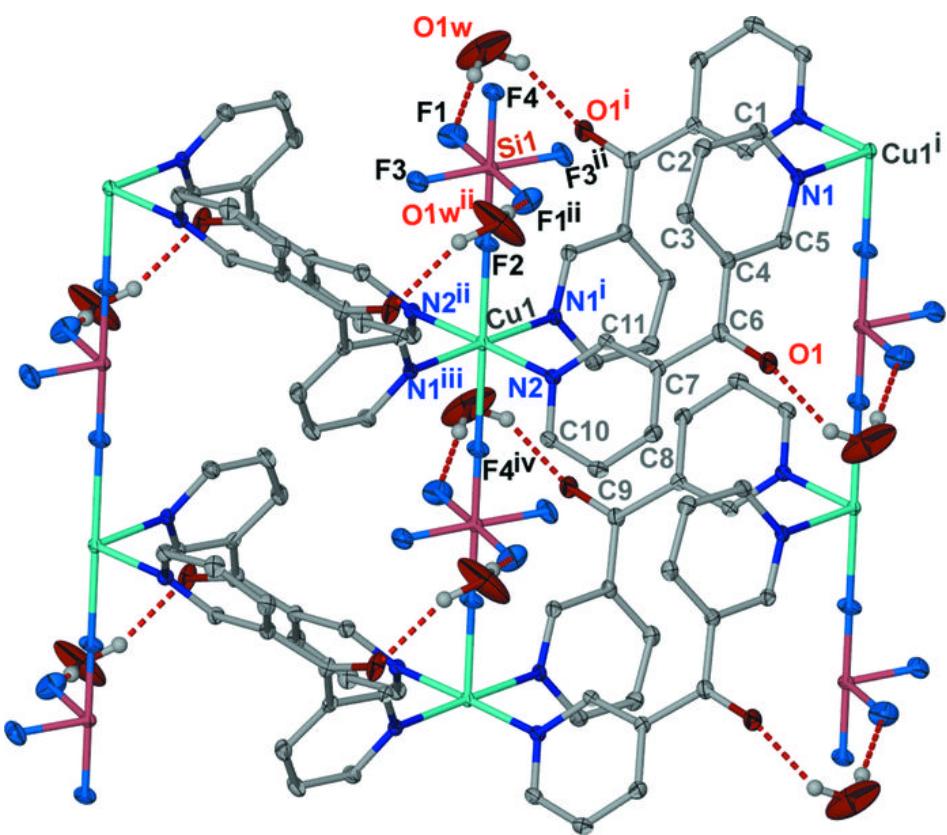
Symmetry codes: (i) $x, -y+1, z-1/2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y, -z+1/2$; (iv) $x, y+1, z$; (v) $x, y-1, z$.

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

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

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

Fig. 1



supplementary materials

Fig. 2

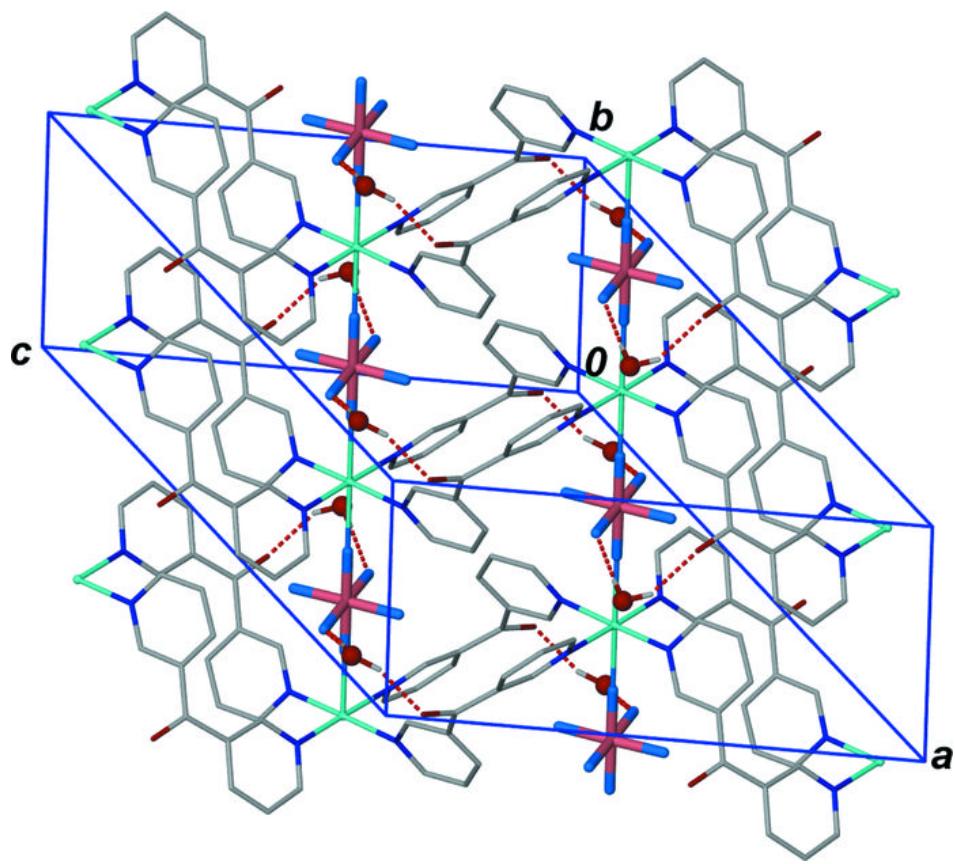


Fig. 3

