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Crystal structures of three copper(II)–2,2′-bipyridine (bpy) compounds, [Cu(bpy)₂(H₂O)]·[SiF₆]·4H₂O, [Cu(bpy)₂(TaF₆)₂] and [Cu(bpy)₃][TaF₆]₂ and a related coordination polymer, [Cu(bpy)(H₂O)₂SnF₆]_n

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We report the hydrothermal syntheses and crystal structures of aquabis(2,2′-bipyridine-κ²N,N′)copper(II) hexafluoridosilicate tetrahydrate, [Cu(bpy)₂(H₂O)]·[SiF₆]·4H₂O (bpy is 2,2′-bipyridine, C₁₀H₈N₂), (I), bis(2,2′-bipyridine-3κ²N,N′)-di-μ-fluorido-1:3κ²F:F;2:3κ²F:F-decafluorido-1κ⁵F,2κ⁵F-ditantalum(V)copper(II), [Cu(bpy)₂(TaF₆)₂], (II), tris(2,2′-bipyridine-κ²N,N′)copper(II) bis[hexafluorido-tantalate(V)], [Cu(bpy)₃][TaF₆]₂, (III), and *catena*-poly[[diaqua(2,2′-bipyridine-κ²N,N′)copper(II)]-μ-fluorido-tetrafluoridotin-μ-fluorido], [Cu(bpy)(H₂O)₂SnF₆]_n, (IV). Compounds (I), (II) and (III) contain locally chiral copper coordination complexes with C₂, D₂, and D₃ symmetry, respectively. The extended structures of (I) and (IV) are consolidated by O–H···F and O–H···O hydrogen bonds. The structure of (III) was found to be a merohedral (racemic) twin.

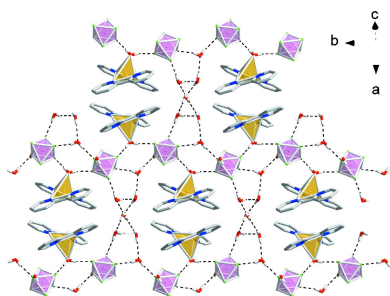
1. Chemical context

Copper(II) complexes of 2,2′-bipyridine (bpy) adopt a wide range of coordination geometries, including square pyramidal, trigonal bipyramidal and octahedral, depending on experimental conditions such as the ligand-to-metal ratio and pH (Garribba *et al.*, 2000). Previous studies have shown that racemic combinations of chiral [Cu(bpy)₂(H₂O)]²⁺ can crystallize in polar structures in the presence of early transition metal fluorides MF₆^{2−}, (M = Ti, Zr, Hf) (Gautier *et al.*, 2012; Nisbet *et al.*, 2020).

Here, we investigate the influence of the anion on the speciation of the copper(II) complex and the arrangement of the ions in the crystal structure in a series of compounds based on copper(II)–2,2′-bipyridine cations and SiF₆^{2−}, SnF₆^{2−} and TaF₆[−] anions. Among these hydrothermally prepared structures we observe three distinct locally chiral copper-bipyridine complexes: C₂-symmetric cations in [Cu(bpy)₂(H₂O)][SiF₆]·4H₂O, (I), D₂-symmetric Cu(bpy)₂(TaF₆)₂ molecules, (II) and D₃-symmetric cations in [Cu(bpy)₃][TaF₆]₂, (III). We also report the structure of a coordination polymer based on Cu(bpy)(H₂O)₂²⁺ cations and SnF₆^{2−} anions, (IV), that forms under similar conditions.

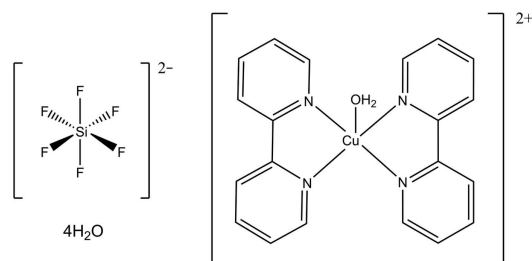
2. Structural commentary

Compound (I) has the formula [Cu(bpy)₂(H₂O)][SiF₆]·4H₂O and crystallizes in space group C2/c. The structure features isolated C₂-symmetric Δ- and Λ-[Cu(bpy)₂(H₂O)]²⁺ cations

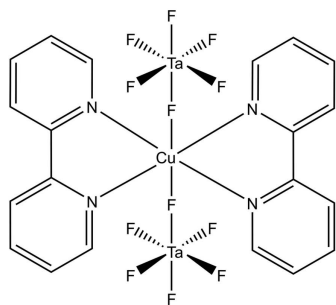


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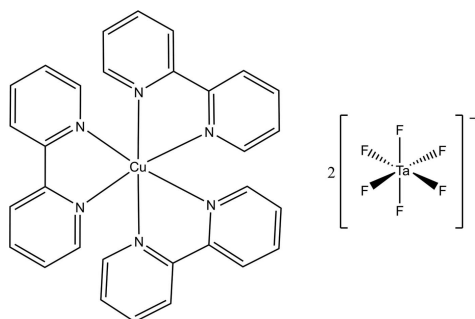
and octahedral SiF_6^{2-} anions (Fig. 1). The five-coordinate Cu^{2+} ion has a slightly distorted trigonal-bipyramidal coordination environment ($\tau = 0.77$), as described by the parameter $\tau = (\beta - \alpha)/60$, where β and α are the two largest angles of the complex ($\tau = 1$ corresponds to an ideal trigonal bipyramid and $\tau = 0$ corresponds to an ideal square pyramid) (Melnic *et al.*, 2014). The average $\text{Cu}-\text{N}$ bond length and the $\text{Cu}-\text{OH}_2$ bond distance in (I) are in agreement with the reported distances in other known $[\text{Cu}(\text{bpy})_2(\text{H}_2\text{O})]^{2+}$ complexes (Gautier *et al.*, 2012; Nisbet *et al.*, 2020; Shi *et al.*, 2010; Yu *et al.*, 2007).



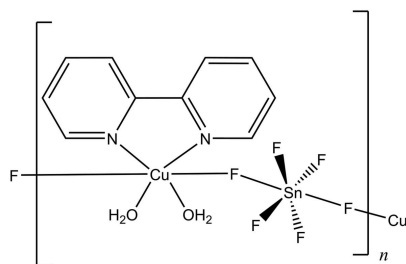
Compound (I)



Compound (II)



Compound (III)



Compound (IV)

Compound (II) has the formula $\text{Cu}(\text{bpy})_2(\text{TaF}_6)_2$ and crystallizes in space group $P\bar{1}$. The structure is comprised of molecular Δ - and Λ - $\text{Cu}(\text{bpy})_2(\text{TaF}_6)_2$ complexes with local D_2

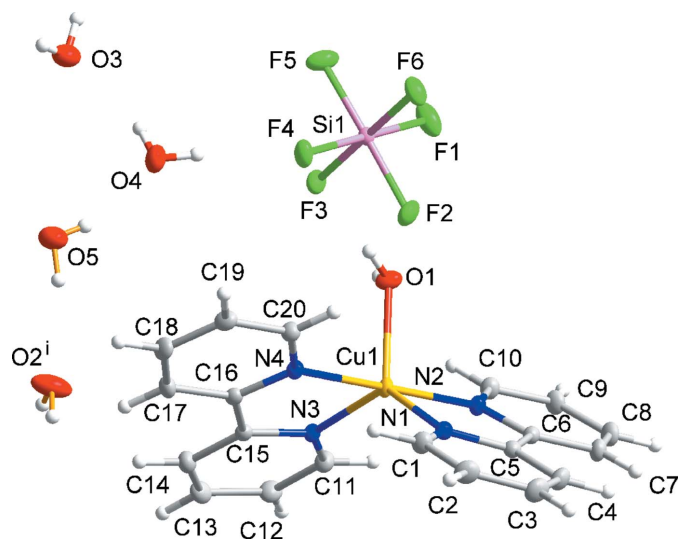


Figure 1

The molecular structure of (I). Ellipsoids of non-H atoms are drawn at 50% probability. H atoms are drawn with an atomic radius of 0.135 Å. [Symmetry code: (i) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$.]

symmetry. Each Cu^{II} center is equatorially coordinated by two bpy ligands and axially coordinated by two TaF_6^- groups. Two independent $\text{Cu}(\text{bpy})_2(\text{TaF}_6)_2$ units with the same handedness are present within the arbitrarily chosen asymmetric unit (Fig. 2). These complexes differ in their $\text{Cu}-\text{F}$ bond lengths and $\text{F}-\text{Cu}-\text{F}$ angles: $\text{Cu1}-\text{F1} = 2.537(3)$, $\text{Cu1}-\text{F7} = 2.987(3)$ Å, $\text{F1}-\text{Cu1}-\text{F7} = 161.46(9)^\circ$; $\text{Cu2}-\text{F13} =$

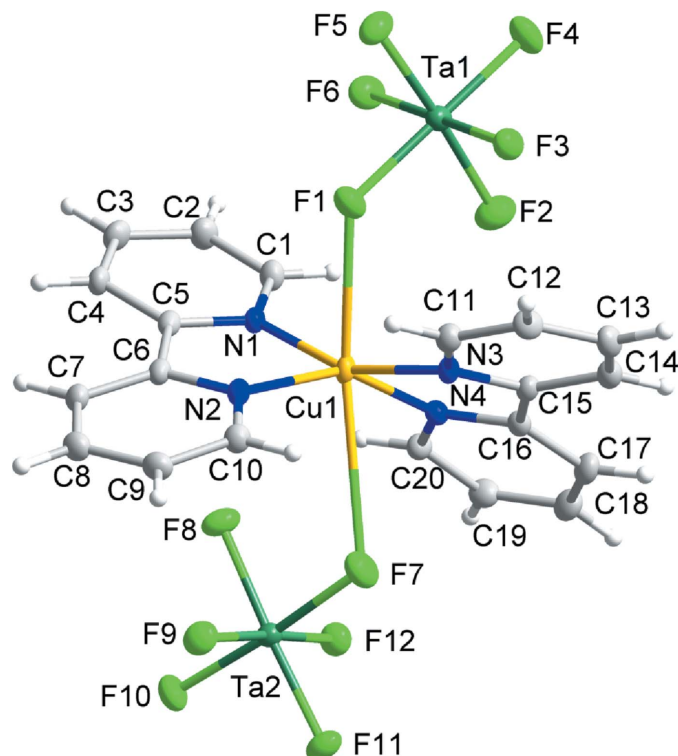


Figure 2

The molecular structure of one of the two independent molecules in (II). Ellipsoids of non-H atoms are drawn at 50% probability. H atoms are drawn with an atomic radius of 0.135 Å.

Table 1
Hydrogen-bond geometry (Å, °) for (I).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1A\cdots F3$	0.76 (3)	1.91 (3)	2.6616 (14)	177 (3)
$O1-H1B\cdots F6^i$	0.78 (2)	1.93 (2)	2.7053 (14)	170 (2)
$O2-H2A\cdots F1$	0.75 (2)	1.94 (2)	2.6677 (17)	164 (2)
$O2-H2B\cdots F4^i$	0.79 (3)	2.00 (3)	2.7807 (17)	167 (2)
$O3-H3A\cdots F5^{ii}$	0.77 (3)	1.99 (3)	2.7607 (18)	177 (3)
$O3-H3B\cdots O5^{iii}$	0.73 (3)	2.06 (3)	2.779 (2)	171 (3)
$O4-H4A\cdots O3$	0.72 (2)	2.05 (2)	2.749 (2)	162 (2)
$O4-H4B\cdots F4$	0.77 (3)	1.98 (3)	2.7462 (16)	170 (2)
$O5-H5A\cdots O4$	0.69 (2)	2.13 (2)	2.779 (2)	158 (2)
$O5-H5B\cdots O2^{iv}$	0.81 (3)	1.99 (3)	2.786 (2)	169 (2)

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

2.706 (3), $Cu2-F19 = 2.775 (3) \text{ \AA}$, $F13-Cu2-F19 = 168.21 (10)^\circ$. The observed Cu—F distances fall above the upper quartile of the distribution of known Cu—F bond distances among structures in the Cambridge Structural Database (mean = 2.240 Å, standard deviation = 0.270 Å). The Cu—N and Cu—F distances in (II) are in reasonable agreement with the bond distances reported in the complex (6,6'-dimethyl-2,2':6',2'':6'',2'''-quaterpyridine)bis(tetrafluoroborate)copper(II) (CSD refcode: UZELOC; Adamski *et al.*, 2017).

Compound (III) has the formula $[Cu(bpy)_3][TaF_6]_2$ and crystallizes in the enantiomorphous space group $P3_2$. The structure of (III) contains D_3 -symmetric Λ - $Cu(bpy)_3^{2+}$ cations with Cu^{II} in an octahedral CuN_6 coordination environment. The Cu—N distances are in agreement with those of the $Cu(bpy)_3^{2+}$ cations in $[Cu(bpy)_3][PF_6]_2$ (CSD refcode:

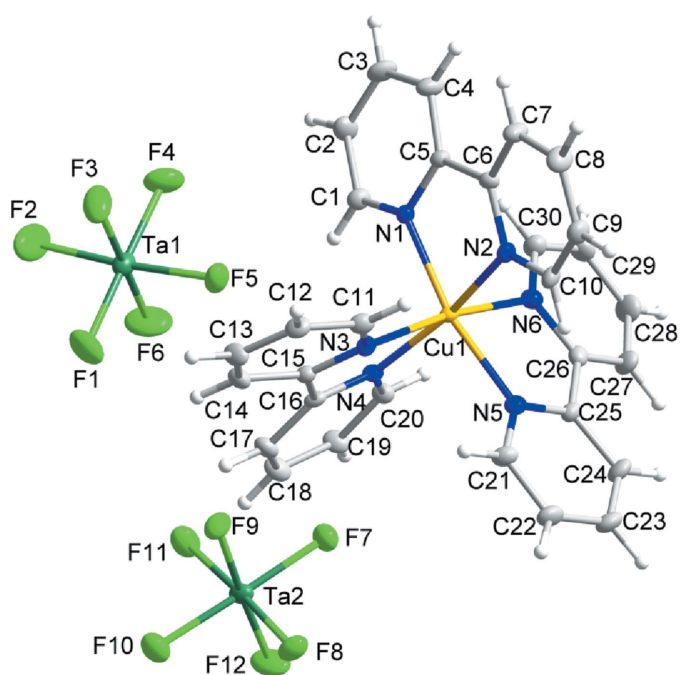


Figure 3
The molecular structure of (III). Ellipsoids of non-H atoms are drawn at 50% probability. H atoms are drawn with an atomic radius of 0.135 Å.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1A\cdots F2^i$	0.88 (3)	1.79 (3)	2.6444 (17)	165 (3)
$O1-H1B\cdots F3^{ii}$	0.81 (3)	1.84 (4)	2.6293 (17)	164 (4)

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

REZJAI; Wang *et al.*, 2007) and $[Cu(bpy)_3][BF_4]_2$ (CSD refcode: RIGTEH; Chamayou *et al.*, 2007). Two distinct octahedral TaF_6^- anions are present in the asymmetric unit (Fig. 3).

Compound (IV) has the formula $Cu(bpy)(H_2O)_2SnF_6$ and crystallizes in space group $P2_1/n$. The structure is composed of one-dimensional coordination chains propagating in the [101] direction that can be described as alternating $Cu(bpy)(H_2O)_2^{2+}$ cations (Cu site symmetry 2) and SnF_6^{2-} anions catenated through bridging Cu—F—Sn linkages. The Sn^{4+} ion occupies a crystallographic inversion center. Intramolecular hydrogen bonding is present along the chains *via* $O1-H1A\cdots F2$ and $O1-H1B\cdots F3$ contacts (Fig. 4; Table 2). The Cu—F bond distance of 2.3830 (10) Å is in agreement with those found in the reported compound $Cu(4,4'$ -bipyridine) $_2SiF_6$ (CSD refcode: PETWES; Nugent *et al.*, 2013).

3. Supramolecular features

In the extended structure of (I), the $Cu(bpy)_2(H_2O)^{2+}$ and SiF_6^{2-} groups are linked *via* $O-H\cdots F$ hydrogen bonding between the apical water molecule and two SiF_6^{2-} ions (Table 1). The Δ/Λ - $Cu(bpy)_2(H_2O)^{2+}$ units participate in displaced heterochiral π - π stacking interactions between the N1/C1–C5 and N2/C6–C10 rings with an interplanar angle of $1.11 (11)^\circ$, centroid–centroid distance of 3.8774 (12) Å, and a slippage distance of 1.490 Å to form Δ up– Λ down– Δ up– Λ down and Δ down– Λ up– Δ down– Λ up chains (up/down

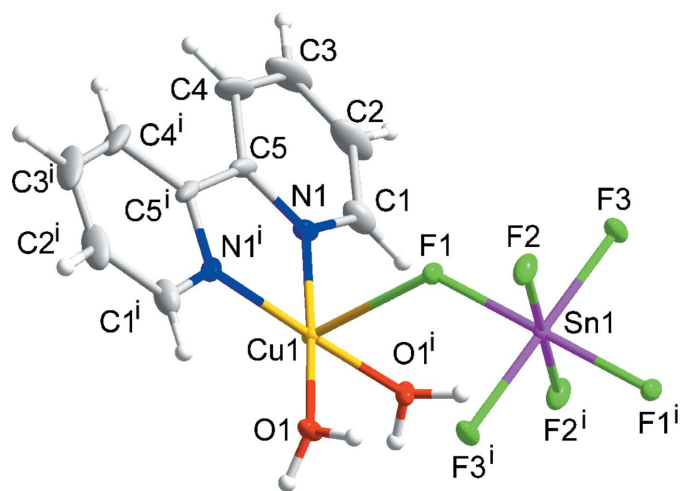


Figure 4
The molecular structure of (IV). Ellipsoids of non-H atoms are drawn at 50% probability. H atoms are drawn with an atomic radius of 0.135 Å. [Symmetry code: (i) $\frac{1}{2} - x, y, \frac{3}{2} - z$.]

refers to the orientation of the Cu—O bond vector in the $+a$ or $-a$ direction). The water molecules of hydration are involved in O—H...F hydrogen bonding interactions with the SiF_6^{2-} anion as well as O—H...O bonds with other water molecules (Fig. 5).

The neutral $\text{Cu}(\text{bpy})_2(\text{TaF}_6)_2$ complexes in (II) form homochiral chains in which the F—Cu—F bond axes of adjacent complexes are aligned along the $a + b$ or $b - a$ directions, as shown in Fig. 6. Along the c -axis direction, each chain is neighbored by a chain with the opposite chirality and same orientation on one side and a chain with the same chirality and opposite orientation on the other.

In (III), the $\Lambda\text{-Cu}(\text{bpy})_3^{2+}$ complexes participate in displaced π – π stacking interactions propagating along the 3_2 screw axes with an interplanar angle of $13.9(2)^\circ$, centroid–centroid distance of $3.933(2) \text{ \AA}$ between adjacent N1/C1–C5 and N5/C21–C25 pyridine rings, and a horizontal shift distance of $1.970 \text{ \AA}$. Each $\Lambda\text{-Cu}(\text{bpy})_3^{2+}$ cation is surrounded by six TaF_6^- anions (Fig. 7).

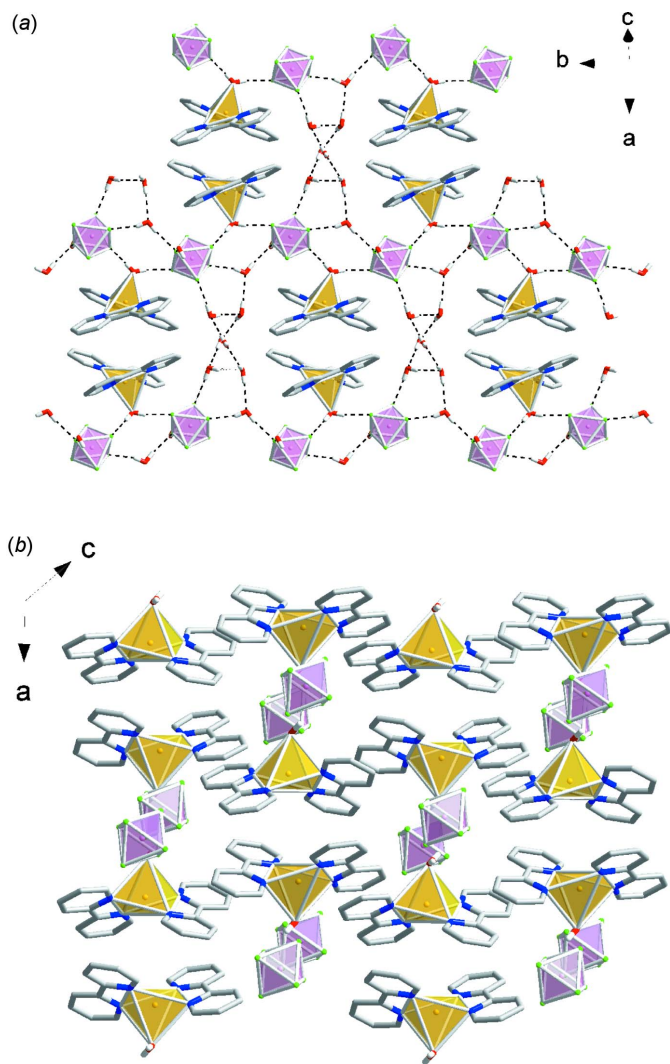


Figure 5
Packing diagram for (I): yellow polyhedra represent $\text{Cu}(\text{bpy})_2(\text{H}_2\text{O})_2^{2+}$ cations and pink polyhedra represent SiF_6^{2-} anions.

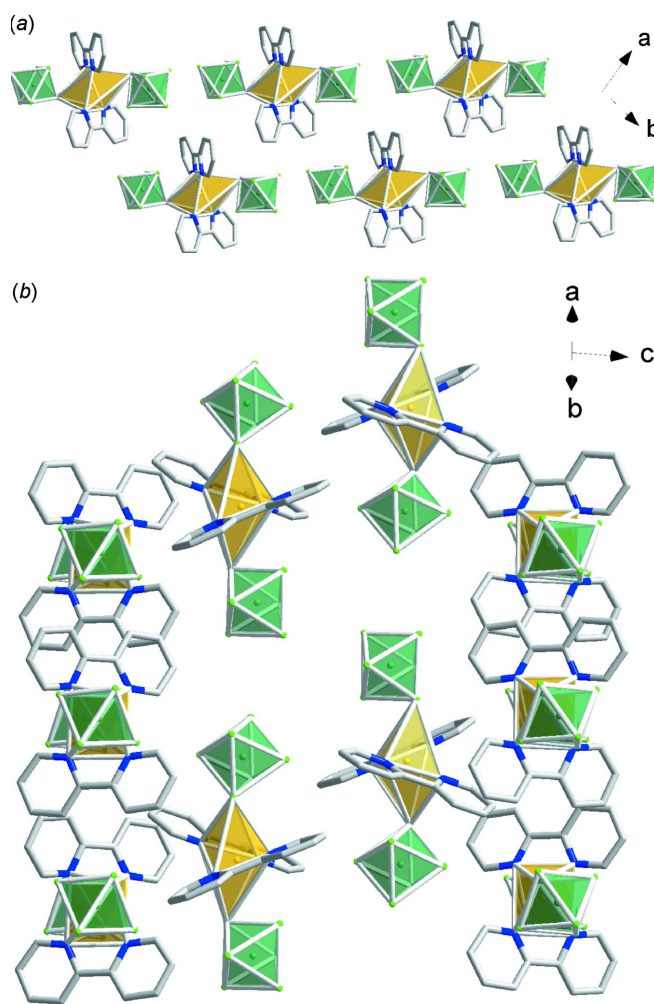


Figure 6
Packing diagram for (II): yellow polyhedra represent $\text{Cu}(\text{bpy})_2^{2+}$ cations and green polyhedra represent TaF_6^- anions.

The one-dimensional coordination chains in (IV) pack in a brickwork arrangement *via* parallel displaced π – π stacking interactions (Fig. 8). One of the stacking interactions involves parallel N1/C1–C5 pyridine rings at a centroid–centroid distance of $3.8133(12) \text{ \AA}$ and a shift distance $1.676 \text{ \AA}$, while the other stacking interaction involves nonparallel N1/C1–C5 pyridine rings with an interplanar angle of $3.54(11)^\circ$, centroid–centroid distance of $3.5830(14) \text{ \AA}$ and a shift distance of $1.072 \text{ \AA}$.

4. Database survey

A survey of structures related to (I) reported in the Cambridge Structural Database (CSD, version 2020.2.0 from September 2020; Groom *et al.*, 2016) produced five other compounds based on $[\text{Cu}(\text{bpy})_2(\text{H}_2\text{O})]^{2+}$ complexes and fluorinated inorganic anions: $[\text{Cu}(\text{bpy})_2(\text{H}_2\text{O})][\text{BF}_4]_2$ (CSD refcode: VIKDOJ; Yu *et al.*, 2007), $[\text{Cu}(\text{bpy})_2(\text{H}_2\text{O})][\text{PF}_6]_2$ (CSD refcode: EQIQOL; Shi *et al.*, 2010), and $[\text{Cu}(\text{bpy})_2(\text{H}_2\text{O})][\text{MF}_6]$ ($M = \text{Ti}, \text{Zr}, \text{Hf}$; CSD refcodes: GESHOD,

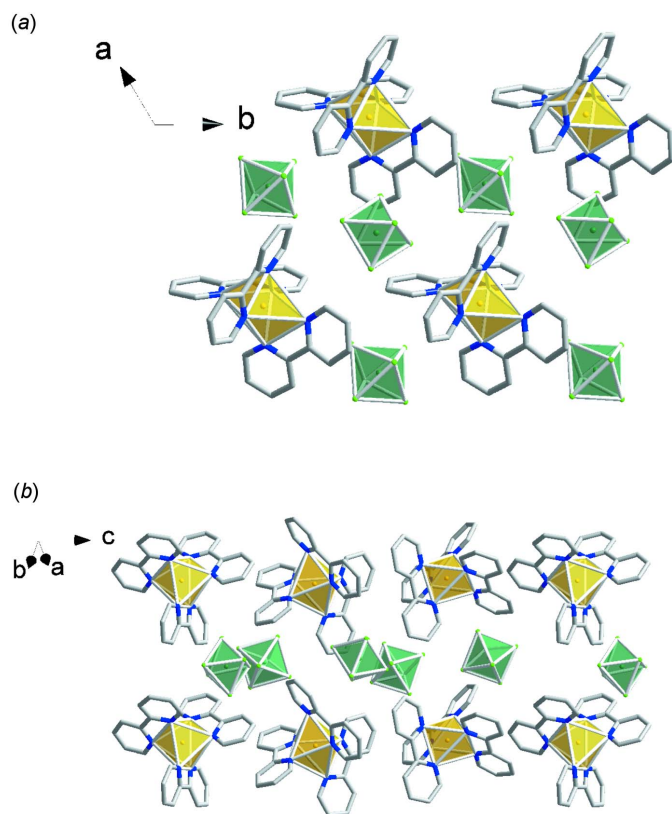


Figure 7
Packing diagram for (III): yellow polyhedra represent $\text{Cu}(\text{bpy})_3^{2+}$ cations and green polyhedra represent TaF_6^{2-} anions.

YUGYEH, YUGYIL, YUGYOR; Gautier *et al.*, 2012; Nisbet *et al.*, 2020). These compounds display a variety of packing architectures, with compounds based on PF_6^- and BF_4^- anions displaying hydrogen-bonded clusters composed of two anions and one cation while compounds based on doubly charged MF_6^{2-} anions form extended hydrogen-bonded networks. The hydrogen-bonding interactions in (I) differ from the analogous compounds based on early transition-metal fluorides in that the MF_6^{2-} anions hydrogen bonded to the $[\text{Cu}(\text{bpy})_2(\text{H}_2\text{O})]^{2+}$ complex are both hydrogen bonded to the same pair of $[\text{Cu}(\text{bpy})_2(\text{H}_2\text{O})]^{2+}$ complexes in the ETM case, whereas they are bound to two different complexes in the SiF_6^{2-} case. Further, while the $[\text{Cu}(\text{bpy})_2(\text{H}_2\text{O})][\text{MF}_6]$ ($M = \text{Ti}, \text{Zr}, \text{Hf}$) compounds display both face-to-face and displaced π - π stacking interactions, (I) has only displaced stacking interactions.

A search of the CSD for structures related to (II) revealed no other known octahedral bis(2,2'-bipyridine)copper(II) complexes with two fluorinated anions coordinated in the apical positions. The most similar example known to the authors is (6,6''-dimethyl-2,2':6',2'':6'',2'''-quaterpyridine)-bis(tetrafluoroborate)copper(II) (CSD refcode: UZELOC; Adamski *et al.*, 2017). This structure features copper(II) complexes arranged such that the F—Cu—F axis of each complex is oriented along the *a*-axis direction. Additionally, these complexes participate in heterochiral π - π stacking interactions.

Compound (III) is a new member of the family of compounds that includes $[\text{A}(\text{bpy})_3][\text{PF}_6]$ ($\text{A} = \text{Mn}, \text{Co}, \text{Ni}, \text{Cu}, \text{Zn}, \text{Ru}$, and Cd ; CSD refcodes: YEGLUR, VUMTEE, WOTSAZ01, REZJAI, WOTSON, BPYRUG, XEFNOM, respectively; (Deisenroth *et al.*, 2001); Breu *et al.*, 2000; Björemark *et al.*, 2015; Wang *et al.*, 2007; Kundu *et al.*, 2005), $\text{Zn}(\text{bpy})_3][\text{TaF}_6]_2$ (CSD refcode: HAHFII; Gautier & Poepelmeier, 2016), and $[\text{Zn}(\text{bpy})_3][\text{NbF}_6]_2$ (CSD refcode: HAHFUI; Gautier & Poepelmeier, 2016). These compounds include either Δ - or Λ - $\text{Cu}(\text{bpy})_3^{2+}$ cations arranged along 3_1 or 3_2 screw axes depending on the handedness of the $\text{Cu}(\text{bpy})_3^{2+}$ complexes.

Compound (IV) is isostructural to the coordination polymer $\text{Cu}(\text{bpy})(\text{H}_2\text{O})\text{HfF}_6$ (CSD refcode: YUGXOQ; Nisbet *et al.*, 2020). These compounds share identical connectivity with a series of coordination polymers with the

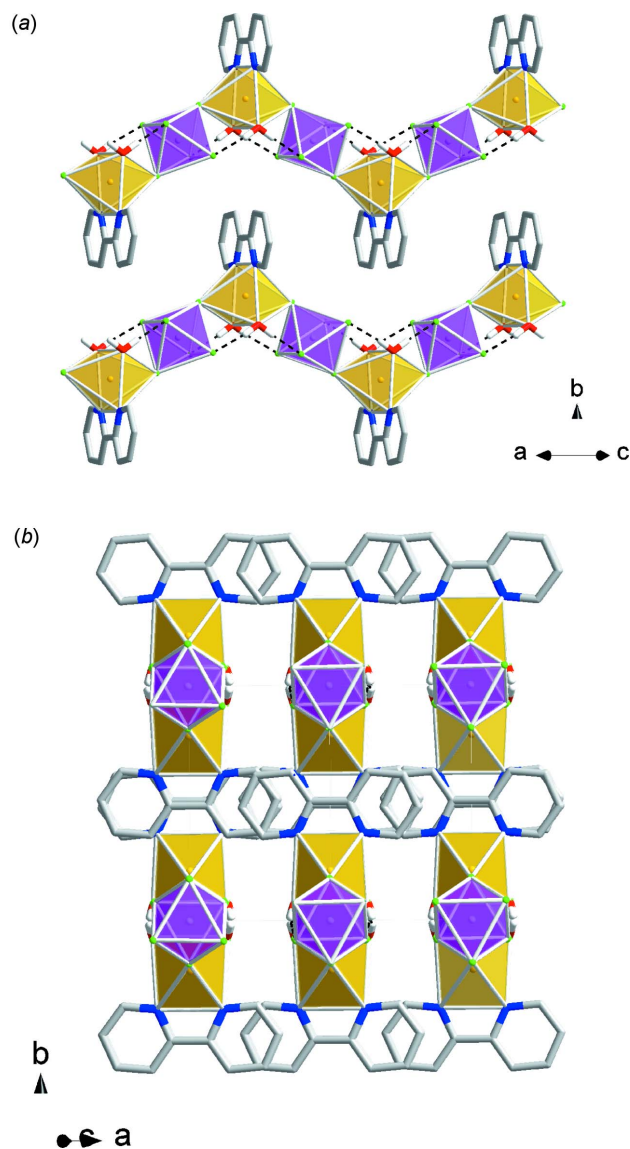


Figure 8
Packing diagram for (IV): Yellow polyhedra represent $\text{Cu}(\text{bpy})(\text{H}_2\text{O})_2^{2+}$ cations and magenta polyhedra represent SnF_6^{2-} anions.

Table 3
Experimental details.

	(I)	(II)	(III)	(IV)
Crystal data				
Chemical formula	[Cu(C ₁₀ H ₈ N ₂) ₂ (H ₂ O)]- [SiF ₆]-4H ₂ O	[CuTa ₂ F ₁₂ (C ₁₀ H ₈ N ₂) ₂]	[Cu(C ₁₀ H ₈ N ₂) ₃][TaF ₆] ₂	[CuSnF ₆ (C ₁₀ H ₈ N ₂)(H ₂ O) ₂]
<i>M_r</i>	608.08	965.81	1121.99	488.45
Crystal system, space group	Monoclinic, <i>C2/c</i>	Triclinic, <i>P</i> $\bar{1}$	Trigonal, <i>P</i> 3 ₂	Monoclinic, <i>P2</i> / <i>n</i>
Temperature (K)	100	100	100	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	25.4971 (16), 13.3573 (9), 18.944 (2)	9.5465 (1), 10.5102 (1), 25.9853 (4)	10.5172 (10), 10.5172 (10), 26.288 (2)	6.2590 (2), 9.2167 (3), 12.1648 (3)
α , β , γ (°)	90, 131.949 (1), 90	96.723 (1), 100.256 (1), 96.672 (1)	90, 90, 120	90, 90.734 (2), 90
<i>V</i> (Å ³)	4798.5 (7)	2522.78 (5)	2518.2 (5)	701.70 (4)
<i>Z</i>	8	4	3	2
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α	Mo <i>K</i> α
μ (mm ⁻¹)	1.05	9.60	7.23	3.37
Crystal size (mm)	0.30 × 0.26 × 0.15	0.52 × 0.32 × 0.22	0.22 × 0.16 × 0.12	0.20 × 0.13 × 0.12
Data collection				
Diffractometer	Bruker APEXII CCD	Rigaku Oxford Diffraction XtaLAB Synergy, Single source at offset/far, HyPix	Bruker Kappa APEX CCD area detector	Rigaku Oxford Diffraction XtaLAB Synergy, Single source at offset/far, HyPix
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2016)	Gaussian <i>CrysAlis PRO</i> (Rigaku OD, 2020)	Multi-scan (<i>SADABS</i> ; Bruker, 2016)	Gaussian <i>CrysAlis PRO</i> (Rigaku OD, 2020)
<i>T</i> _{min} , <i>T</i> _{max}	0.694, 0.746	0.035, 0.414	0.559, 0.746	0.732, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	57770, 6660, 5863	93570, 18263, 15170	148130, 12260, 12121	22131, 3686, 3251
<i>R</i> _{int}	0.050	0.060	0.050	0.055
(sin θ /λ) _{max} (Å ⁻¹)	0.693	0.785	0.761	0.870
Refinement				
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.027, 0.070, 1.04	0.037, 0.088, 1.05	0.016, 0.031, 1.03	0.029, 0.067, 1.07
No. of reflections	6660	18263	12260	3686
No. of parameters	374	704	462	110
No. of restraints	0	0	1	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.79, -0.25	1.67, -3.53	0.96, -0.85	2.05, -0.85
Absolute structure	—	—	Flack <i>x</i> determined using 5861 quotients [(<i>I</i> ⁺) - (<i>I</i> ⁻)]/ [(<i>I</i> ⁺) + (<i>I</i> ⁻)] (Parsons <i>et al.</i> , 2013)	—
Absolute structure parameter	—	—	0.5036 (7)	—

Computer programs: *APEX2* (Bruker, 2017), *SAINT* (Bruker, 2016), *CrysAlis PRO* (Rigaku OD, 2020), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), and *OLEX2* (Dolomanov *et al.*, 2009).

formula *M'*(bpy)(H₂O)₂MO_xF_{6-x} compounds (*M*/*M* = Cu/Ti, Cu/V, Cu/Nb, Cu/Mo, Zn/Mo, and Zn/W), which display polar zigzag chains (Gautier & Poeppelmeier, 2013).

5. Synthesis and crystallization

The compounds reported here were synthesized by the hydrothermal pouch method (Harrison *et al.*, 1993). In each reaction, reagents were heat sealed in Teflon pouches. Groups of six pouches were then placed into a 125 ml Parr autoclave with 40 ml distilled water as backfill. The autoclave was heated at a rate of 5°C min⁻¹ to 150°C and held at 150°C for 24 h. The autoclaves were allowed to cool to room temperature at a rate of 6°C h⁻¹ and the solid products were recovered by vacuum filtration. Compound (I) was synthesized in a pouch containing 1.9 mmol of Cu(NO₃)₂·H₂O, 5 mmol of 2,2'-bipyridine, 1.5 mmol of (NH₄)₂SiF₆ and 1 ml of deionized H₂O.

Compound (II) was synthesized in a pouch containing 1.7 mmol of CuO, 2.5 mmol of 2,2'-bipyridine, 0.85 mmol of Ta₂O₅, 0.8 ml HF(aq), and 0.3 ml of deionized H₂O. Compound (III) was synthesized in a pouch containing 1.7 mmol of CuO, 5.1 mmol of 2,2'-bipyridine, 0.85 mmol Ta₂O₅, 1 ml of HF(aq) and 0.1 ml of deionized H₂O. Compound (IV) was synthesized in a pouch containing 1.9 mmol of Cu(NO₃)₂·H₂O, 1.3 mmol of 2,2'-bipyridine, 1.7 mmol of (NH₄)₂SnF₆ and 1 ml of deionized H₂O.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atom positions were assigned from difference map peaks and their positions freely refined with the exception of C—H hydrogen atoms of

2,2'-bipyridine, which were constrained to ride at distances of 0.95 Å from the associated C atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

The measured crystal of (III) is a class II twin by merohedry about a twofold axis along the [110] direction to give apparent Laue symmetry of $\bar{3}m1$. The twinning occurs with a BASF of 0.5, suggesting that both the $P3_1$ and $P3_2$ configurations are present in equal proportions within the sample.

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supporting information

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Crystal structures of three copper(II)–2,2'-bipyridine (bpy) compounds, [Cu(bpy)₂(H₂O)][SiF₆]·4H₂O, [Cu(bpy)₂(TaF₆)₂] and [Cu(bpy)₃][TaF₆]₂ and a related coordination polymer, [Cu(bpy)(H₂O)₂SnF₆]_n

Matthew L. Nisbet, Emily Hiralal and Kenneth R. Poeppelmeier

Computing details

Data collection: *APEX2* (Bruker, 2017) for (I), (III); *CrysAlis PRO* (Rigaku OD, 2020) for (II), (IV). Cell refinement: *SAINT* (Bruker, 2016) for (I), (III); *CrysAlis PRO* (Rigaku OD, 2020) for (II), (IV). Data reduction: *SAINT* (Bruker, 2016) for (I), (III); *CrysAlis PRO* (Rigaku OD, 2020) for (II), (IV). For all structures, program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Aquabis(2,2'-bipyridine- κ^2N,N')copper(II) hexafluorosilicate tetrahydrate (I)

Crystal data

[Cu(C₁₀H₈N₂)₂(H₂O)][SiF₆]·4H₂O
 M_r = 608.08
 Monoclinic, *C2/c*
 a = 25.4971 (16) Å
 b = 13.3573 (9) Å
 c = 18.944 (2) Å
 β = 131.949 (1)°
 V = 4798.5 (7) Å³
 Z = 8

$F(000)$ = 2488
 D_x = 1.683 Mg m⁻³
 Mo $K\alpha$ radiation, λ = 0.71073 Å
 Cell parameters from 9731 reflections
 θ = 2.8–29.4°
 μ = 1.05 mm⁻¹
 T = 100 K
 Block, blue
 0.30 × 0.26 × 0.15 mm

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: sealed tube
 Triumph monochromator
 Detector resolution: 8 pixels mm⁻¹
 ϕ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2016)
 $T_{\min}$ = 0.694, $T_{\max}$ = 0.746

57770 measured reflections
 6660 independent reflections
 5863 reflections with $I > 2\sigma(I)$
 R_{int} = 0.050
 θ_{max} = 29.5°, θ_{min} = 1.9°
 h = -35→34
 k = -18→18
 l = -24→26

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)]$ = 0.027
 $wR(F^2)$ = 0.070
 S = 1.04
 6660 reflections

374 parameters
 0 restraints
 Primary atom site location: dual
 Hydrogen site location: mixed
 H atoms treated by a mixture of independent
 and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 6.982P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.79 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$$

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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.38373 (2)	0.37571 (2)	0.22886 (2)	0.01115 (5)
O1	0.30718 (6)	0.41614 (9)	0.23571 (8)	0.0177 (2)
H1A	0.3036 (13)	0.3839 (18)	0.2650 (17)	0.035 (6)*
H1B	0.3081 (12)	0.4726 (19)	0.2479 (16)	0.033 (6)*
N1	0.37806 (6)	0.26410 (8)	0.15033 (8)	0.0120 (2)
N3	0.46003 (6)	0.48439 (9)	0.31770 (8)	0.0122 (2)
N4	0.44106 (6)	0.30358 (8)	0.35115 (8)	0.0124 (2)
N2	0.32619 (6)	0.44426 (9)	0.10503 (8)	0.0124 (2)
C6	0.31103 (7)	0.39110 (10)	0.03265 (9)	0.0117 (2)
C16	0.49954 (7)	0.35110 (10)	0.42717 (9)	0.0122 (2)
C15	0.51060 (7)	0.45257 (10)	0.40829 (9)	0.0120 (2)
C17	0.54345 (8)	0.30770 (11)	0.51640 (10)	0.0164 (3)
H17	0.584712	0.341450	0.569103	0.020*
C4	0.33051 (8)	0.22242 (11)	−0.00601 (10)	0.0166 (3)
H4	0.303744	0.241407	−0.070316	0.020*
C5	0.34040 (7)	0.28885 (10)	0.05837 (9)	0.0120 (2)
C11	0.46479 (8)	0.57742 (10)	0.29641 (10)	0.0156 (3)
H11	0.429070	0.600245	0.233009	0.019*
C18	0.52625 (8)	0.21425 (11)	0.52759 (10)	0.0181 (3)
H18	0.555859	0.183054	0.588184	0.022*
C12	0.51911 (8)	0.64187 (11)	0.36212 (11)	0.0177 (3)
H12	0.520466	0.707626	0.344271	0.021*
C20	0.42436 (8)	0.21398 (10)	0.36308 (10)	0.0149 (3)
H20	0.382534	0.181730	0.309805	0.018*
C14	0.56701 (8)	0.51293 (11)	0.47781 (10)	0.0168 (3)
H14	0.602223	0.488785	0.540838	0.020*
C19	0.46602 (8)	0.16686 (11)	0.45043 (10)	0.0165 (3)
H19	0.453313	0.103009	0.457052	0.020*
C10	0.30008 (8)	0.53675 (10)	0.08876 (10)	0.0151 (3)
H10	0.309292	0.572663	0.139338	0.018*
C3	0.36042 (9)	0.12784 (11)	0.02521 (11)	0.0197 (3)
H3	0.353934	0.080777	−0.017661	0.024*
C2	0.39978 (9)	0.10290 (11)	0.11951 (11)	0.0192 (3)
H2	0.421146	0.038806	0.142568	0.023*
C9	0.26007 (8)	0.58174 (11)	0.00054 (10)	0.0165 (3)
H9	0.242705	0.647922	−0.009131	0.020*

C13	0.57152 (8)	0.60901 (11)	0.45437 (11)	0.0187 (3)
H13	0.609914	0.651426	0.500877	0.022*
C7	0.27095 (8)	0.43169 (11)	−0.05742 (10)	0.0159 (3)
H7	0.260819	0.393583	−0.107643	0.019*
C1	0.40748 (8)	0.17297 (10)	0.17963 (10)	0.0158 (3)
H1	0.434783	0.155761	0.244450	0.019*
C8	0.24582 (8)	0.52859 (11)	−0.07328 (10)	0.0178 (3)
H8	0.219083	0.558236	−0.134231	0.021*
Si1	0.23943 (2)	0.20875 (3)	0.28568 (3)	0.01040 (8)
F4	0.30094 (5)	0.12511 (7)	0.36761 (6)	0.02014 (19)
F2	0.26224 (5)	0.18737 (8)	0.22236 (6)	0.0246 (2)
F6	0.17998 (5)	0.11481 (6)	0.22816 (6)	0.02098 (19)
F3	0.30005 (5)	0.30181 (7)	0.34414 (6)	0.01928 (18)
F5	0.21850 (6)	0.23088 (7)	0.35102 (8)	0.0248 (2)
F1	0.17872 (5)	0.29058 (7)	0.20409 (7)	0.0281 (2)
O2	0.14362 (8)	0.48395 (10)	0.17503 (12)	0.0332 (3)
H2A	0.1591 (11)	0.4330 (17)	0.1834 (15)	0.023 (5)*
H2B	0.1657 (13)	0.5213 (19)	0.1710 (17)	0.036 (6)*
O3	0.39995 (8)	0.19743 (10)	0.68756 (10)	0.0252 (3)
H3A	0.3668 (14)	0.2152 (18)	0.6774 (17)	0.037 (7)*
H3B	0.4124 (14)	0.156 (2)	0.7206 (19)	0.046 (8)*
O4	0.41008 (7)	0.12569 (10)	0.56108 (9)	0.0246 (3)
H4A	0.3995 (12)	0.1479 (17)	0.5847 (16)	0.028 (6)*
H4B	0.3776 (14)	0.1313 (17)	0.5077 (19)	0.036 (7)*
O5	0.54187 (8)	0.03556 (10)	0.68866 (10)	0.0267 (3)
H5A	0.5100 (11)	0.0531 (15)	0.6479 (15)	0.013 (5)*
H5B	0.5669 (13)	0.0274 (18)	0.6773 (17)	0.040 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01351 (9)	0.00970 (8)	0.00754 (8)	0.00123 (6)	0.00592 (7)	0.00124 (5)
O1	0.0241 (6)	0.0120 (5)	0.0260 (6)	0.0011 (4)	0.0205 (5)	0.0028 (4)
N1	0.0122 (6)	0.0115 (5)	0.0113 (5)	0.0010 (4)	0.0075 (5)	0.0002 (4)
N3	0.0126 (6)	0.0127 (5)	0.0104 (5)	−0.0005 (4)	0.0074 (5)	0.0006 (4)
N4	0.0132 (6)	0.0124 (5)	0.0110 (5)	0.0015 (4)	0.0078 (5)	0.0019 (4)
N2	0.0138 (6)	0.0115 (5)	0.0103 (5)	0.0019 (4)	0.0074 (5)	0.0009 (4)
C6	0.0118 (6)	0.0125 (6)	0.0107 (6)	−0.0002 (5)	0.0074 (5)	0.0001 (5)
C16	0.0122 (6)	0.0132 (6)	0.0121 (6)	0.0020 (5)	0.0085 (5)	0.0014 (5)
C15	0.0117 (6)	0.0136 (6)	0.0115 (6)	0.0010 (5)	0.0080 (5)	0.0006 (5)
C17	0.0128 (7)	0.0194 (7)	0.0114 (6)	0.0012 (5)	0.0058 (6)	0.0015 (5)
C4	0.0212 (8)	0.0165 (6)	0.0141 (6)	0.0005 (5)	0.0126 (6)	−0.0010 (5)
C5	0.0116 (6)	0.0122 (6)	0.0118 (6)	0.0000 (5)	0.0078 (5)	0.0004 (5)
C11	0.0179 (7)	0.0141 (6)	0.0144 (6)	−0.0008 (5)	0.0105 (6)	0.0016 (5)
C18	0.0171 (7)	0.0211 (7)	0.0134 (6)	0.0056 (5)	0.0090 (6)	0.0078 (5)
C12	0.0206 (7)	0.0137 (6)	0.0201 (7)	−0.0039 (5)	0.0141 (6)	−0.0014 (5)
C20	0.0151 (7)	0.0151 (6)	0.0142 (6)	0.0003 (5)	0.0097 (6)	0.0015 (5)
C14	0.0145 (7)	0.0189 (7)	0.0130 (6)	−0.0010 (5)	0.0075 (6)	−0.0011 (5)

C19	0.0193 (7)	0.0146 (6)	0.0191 (7)	0.0033 (5)	0.0142 (6)	0.0049 (5)
C10	0.0170 (7)	0.0129 (6)	0.0138 (6)	0.0017 (5)	0.0097 (6)	0.0004 (5)
C3	0.0268 (8)	0.0155 (6)	0.0216 (7)	0.0002 (6)	0.0181 (7)	−0.0038 (5)
C2	0.0240 (8)	0.0133 (6)	0.0241 (7)	0.0044 (5)	0.0177 (7)	0.0011 (5)
C9	0.0169 (7)	0.0136 (6)	0.0144 (6)	0.0041 (5)	0.0085 (6)	0.0037 (5)
C13	0.0166 (7)	0.0188 (7)	0.0181 (7)	−0.0049 (5)	0.0105 (6)	−0.0053 (5)
C7	0.0167 (7)	0.0179 (6)	0.0103 (6)	0.0007 (5)	0.0078 (6)	0.0006 (5)
C1	0.0178 (7)	0.0133 (6)	0.0159 (6)	0.0037 (5)	0.0111 (6)	0.0029 (5)
C8	0.0177 (7)	0.0183 (7)	0.0123 (6)	0.0033 (5)	0.0080 (6)	0.0047 (5)
Si1	0.01073 (18)	0.00884 (15)	0.00999 (16)	0.00026 (13)	0.00624 (15)	0.00056 (12)
F4	0.0190 (5)	0.0192 (4)	0.0132 (4)	0.0048 (3)	0.0070 (4)	0.0019 (3)
F2	0.0299 (5)	0.0312 (5)	0.0166 (4)	−0.0035 (4)	0.0171 (4)	−0.0048 (4)
F6	0.0171 (4)	0.0126 (4)	0.0194 (4)	−0.0030 (3)	0.0065 (4)	0.0002 (3)
F3	0.0205 (5)	0.0198 (4)	0.0144 (4)	−0.0078 (3)	0.0103 (4)	−0.0032 (3)
F5	0.0360 (6)	0.0175 (4)	0.0397 (6)	−0.0025 (4)	0.0331 (5)	−0.0043 (4)
F1	0.0198 (5)	0.0147 (4)	0.0271 (5)	0.0010 (4)	0.0063 (4)	0.0065 (4)
O2	0.0311 (7)	0.0166 (6)	0.0643 (10)	0.0028 (5)	0.0371 (8)	0.0061 (6)
O3	0.0239 (7)	0.0252 (6)	0.0312 (7)	−0.0023 (5)	0.0204 (6)	−0.0025 (5)
O4	0.0253 (7)	0.0281 (6)	0.0154 (6)	−0.0004 (5)	0.0116 (6)	0.0012 (5)
O5	0.0242 (7)	0.0280 (6)	0.0323 (7)	0.0018 (5)	0.0207 (7)	0.0037 (5)

Geometric parameters (Å, °)

Cu1—O1	2.1112 (11)	C20—C19	1.3831 (19)
Cu1—N1	2.0419 (12)	C14—H14	0.9500
Cu1—N3	2.0849 (12)	C14—C13	1.388 (2)
Cu1—N4	1.9760 (11)	C19—H19	0.9500
Cu1—N2	1.9730 (11)	C10—H10	0.9500
O1—H1A	0.76 (3)	C10—C9	1.3841 (19)
O1—H1B	0.78 (2)	C3—H3	0.9500
N1—C5	1.3527 (17)	C3—C2	1.383 (2)
N1—C1	1.3401 (17)	C2—H2	0.9500
N3—C15	1.3528 (17)	C2—C1	1.383 (2)
N3—C11	1.3368 (17)	C9—H9	0.9500
N4—C16	1.3525 (18)	C9—C8	1.383 (2)
N4—C20	1.3392 (18)	C13—H13	0.9500
N2—C6	1.3510 (17)	C7—H7	0.9500
N2—C10	1.3379 (18)	C7—C8	1.385 (2)
C6—C5	1.4749 (18)	C1—H1	0.9500
C6—C7	1.3852 (18)	C8—H8	0.9500
C16—C15	1.4761 (19)	Si1—F4	1.6918 (9)
C16—C17	1.3845 (19)	Si1—F2	1.6708 (10)
C15—C14	1.3860 (19)	Si1—F6	1.6886 (9)
C17—H17	0.9500	Si1—F3	1.6947 (9)
C17—C18	1.386 (2)	Si1—F5	1.6695 (10)
C4—H4	0.9500	Si1—F1	1.6677 (10)
C4—C5	1.3883 (19)	O2—H2A	0.75 (2)
C4—C3	1.387 (2)	O2—H2B	0.79 (3)

C11—H11	0.9500	O3—H3A	0.77 (3)
C11—C12	1.380 (2)	O3—H3B	0.73 (3)
C18—H18	0.9500	O4—H4A	0.72 (2)
C18—C19	1.376 (2)	O4—H4B	0.77 (3)
C12—H12	0.9500	O5—H5A	0.69 (2)
C12—C13	1.382 (2)	O5—H5B	0.81 (3)
C20—H20	0.9500		
N1—Cu1—O1	127.84 (5)	N4—C20—H20	118.9
N1—Cu1—N3	132.07 (5)	N4—C20—C19	122.15 (14)
N3—Cu1—O1	100.04 (5)	C19—C20—H20	118.9
N4—Cu1—O1	92.43 (5)	C15—C14—H14	120.4
N4—Cu1—N1	97.75 (5)	C15—C14—C13	119.29 (13)
N4—Cu1—N3	80.40 (5)	C13—C14—H14	120.4
N2—Cu1—O1	88.34 (5)	C18—C19—C20	118.74 (13)
N2—Cu1—N1	80.70 (5)	C18—C19—H19	120.6
N2—Cu1—N3	100.81 (5)	C20—C19—H19	120.6
N2—Cu1—N4	178.43 (5)	N2—C10—H10	119.0
Cu1—O1—H1A	118.2 (18)	N2—C10—C9	122.06 (13)
Cu1—O1—H1B	114.6 (17)	C9—C10—H10	119.0
H1A—O1—H1B	109 (2)	C4—C3—H3	120.4
C5—N1—Cu1	113.79 (9)	C2—C3—C4	119.18 (13)
C1—N1—Cu1	127.88 (10)	C2—C3—H3	120.4
C1—N1—C5	118.32 (12)	C3—C2—H2	120.6
C15—N3—Cu1	112.90 (9)	C1—C2—C3	118.80 (14)
C11—N3—Cu1	128.87 (10)	C1—C2—H2	120.6
C11—N3—C15	118.23 (12)	C10—C9—H9	120.6
C16—N4—Cu1	116.39 (9)	C8—C9—C10	118.78 (13)
C20—N4—Cu1	124.34 (10)	C8—C9—H9	120.6
C20—N4—C16	119.23 (12)	C12—C13—C14	118.78 (14)
C6—N2—Cu1	116.33 (9)	C12—C13—H13	120.6
C10—N2—Cu1	124.23 (9)	C14—C13—H13	120.6
C10—N2—C6	119.40 (12)	C6—C7—H7	120.4
N2—C6—C5	114.45 (11)	C6—C7—C8	119.10 (13)
N2—C6—C7	121.29 (12)	C8—C7—H7	120.4
C7—C6—C5	124.26 (12)	N1—C1—C2	122.79 (13)
N4—C16—C15	115.22 (12)	N1—C1—H1	118.6
N4—C16—C17	121.31 (13)	C2—C1—H1	118.6
C17—C16—C15	123.42 (13)	C9—C8—C7	119.32 (13)
N3—C15—C16	114.92 (12)	C9—C8—H8	120.3
N3—C15—C14	121.76 (13)	C7—C8—H8	120.3
C14—C15—C16	123.29 (12)	F4—Si1—F3	90.21 (5)
C16—C17—H17	120.5	F2—Si1—F4	89.52 (5)
C16—C17—C18	118.93 (14)	F2—Si1—F6	90.16 (5)
C18—C17—H17	120.5	F2—Si1—F3	89.51 (5)
C5—C4—H4	120.6	F6—Si1—F4	89.03 (5)
C3—C4—H4	120.6	F6—Si1—F3	179.18 (5)
C3—C4—C5	118.83 (13)	F5—Si1—F4	89.80 (5)

N1—C5—C6	114.73 (11)	F5—Si1—F2	178.71 (6)
N1—C5—C4	122.06 (13)	F5—Si1—F6	90.92 (5)
C4—C5—C6	123.21 (12)	F5—Si1—F3	89.40 (5)
N3—C11—H11	118.4	F1—Si1—F4	179.43 (6)
N3—C11—C12	123.13 (13)	F1—Si1—F2	89.97 (6)
C12—C11—H11	118.4	F1—Si1—F6	90.70 (5)
C17—C18—H18	120.2	F1—Si1—F3	90.05 (5)
C19—C18—C17	119.62 (13)	F1—Si1—F5	90.71 (6)
C19—C18—H18	120.2	H2A—O2—H2B	106 (2)
C11—C12—H12	120.6	H3A—O3—H3B	103 (3)
C11—C12—C13	118.79 (13)	H4A—O4—H4B	105 (2)
C13—C12—H12	120.6	H5A—O5—H5B	107 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1A...F3	0.76 (3)	1.91 (3)	2.6616 (14)	177 (3)
O1—H1B...F6 ⁱ	0.78 (2)	1.93 (2)	2.7053 (14)	170 (2)
O2—H2A...F1	0.75 (2)	1.94 (2)	2.6677 (17)	164 (2)
O2—H2B...F4 ⁱ	0.79 (3)	2.00 (3)	2.7807 (17)	167 (2)
O3—H3A...F5 ⁱⁱ	0.77 (3)	1.99 (3)	2.7607 (18)	177 (3)
O3—H3B...O5 ⁱⁱⁱ	0.73 (3)	2.06 (3)	2.779 (2)	171 (3)
O4—H4A...O3	0.72 (2)	2.05 (2)	2.749 (2)	162 (2)
O4—H4B...F4	0.77 (3)	1.98 (3)	2.7462 (16)	170 (2)
O5—H5A...O4	0.69 (2)	2.13 (2)	2.779 (2)	158 (2)
O5—H5B...O2 ^{iv}	0.81 (3)	1.99 (3)	2.786 (2)	169 (2)

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

Bis(2,2'-bipyridine-3 κ^2 N,N')-di- μ -fluorido-1:3 κ^2 F:F;2:3 κ^2 F:F-decafluorido-1 κ^5 F,2 κ^5 F-copper(II)ditantalum(V) (II)*Crystal data*[CuTa₂F₁₂(C₁₀H₈N₂)₂] $M_r = 965.81$ Triclinic, $P\bar{1}$ $a = 9.5465$ (1) Å $b = 10.5102$ (1) Å $c = 25.9853$ (4) Å $\alpha = 96.723$ (1)° $\beta = 100.256$ (1)° $\gamma = 96.672$ (1)° $V = 2522.78$ (5) Å³ $Z = 4$ $F(000) = 1788$ $D_x = 2.543$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 52090 reflections

 $\theta = 2.1$ – 33.9 ° $\mu = 9.60$ mm⁻¹ $T = 100$ K

Plate, blue

 $0.52 \times 0.32 \times 0.22$ mm*Data collection*

Rigaku Oxford Diffraction XtaLAB Synergy,

Single source at offset/far, HyPix

diffractometer

Radiation source: micro-focus sealed X-ray

tube, PhotonJet (Mo) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹ ω scans

Absorption correction: gaussian

CrysAlispro (Rigaku OD, 2020)

 $T_{\min} = 0.035$, $T_{\max} = 0.414$

93570 measured reflections

18263 independent reflections

15170 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.060$ $\theta_{\max} = 33.9$ °, $\theta_{\min} = 2.0$ °

$h = -14 \rightarrow 13$
 $k = -16 \rightarrow 16$

$l = -40 \rightarrow 39$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.088$
 $S = 1.05$
 18263 reflections
 704 parameters
 0 restraints
 Hydrogen site location: inferred from
 neighbouring sites

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 5.1565P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 1.67 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -3.53 \text{ e } \text{\AA}^{-3}$
 Extinction correction: SHELXL-2018/3
 (Sheldrick 2015b),
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00034 (4)

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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ta2	0.98596 (2)	1.10178 (2)	0.12906 (2)	0.01573 (4)
Ta1	0.41338 (2)	0.45975 (2)	0.10819 (2)	0.01761 (4)
Cu1	0.68618 (5)	0.78568 (5)	0.13192 (2)	0.01516 (9)
F9	0.9510 (3)	1.1887 (3)	0.19295 (10)	0.0252 (5)
F5	0.2489 (3)	0.4552 (3)	0.14002 (11)	0.0267 (6)
F8	0.7872 (3)	1.0564 (3)	0.10038 (11)	0.0260 (6)
F12	1.0286 (3)	1.0247 (3)	0.06509 (10)	0.0239 (5)
F11	1.1860 (3)	1.1389 (3)	0.15719 (11)	0.0262 (6)
F3	0.5185 (3)	0.4088 (3)	0.16953 (11)	0.0247 (5)
F7	0.9770 (3)	0.9436 (3)	0.15757 (11)	0.0294 (6)
F4	0.3621 (3)	0.2852 (3)	0.07704 (12)	0.0305 (6)
F10	0.9810 (3)	1.2592 (2)	0.10011 (11)	0.0256 (6)
F2	0.5792 (3)	0.4746 (3)	0.07763 (12)	0.0331 (6)
F6	0.3068 (3)	0.5133 (3)	0.04785 (11)	0.0270 (6)
F1	0.4651 (3)	0.6364 (2)	0.14024 (11)	0.0269 (6)
N3	0.7804 (4)	0.6735 (3)	0.17963 (14)	0.0160 (6)
N1	0.5349 (3)	0.8408 (3)	0.08062 (14)	0.0157 (6)
N4	0.8057 (4)	0.7153 (3)	0.08444 (14)	0.0152 (6)
N2	0.6440 (4)	0.9307 (3)	0.17981 (14)	0.0157 (6)
C2	0.3580 (5)	0.8158 (4)	0.00134 (18)	0.0216 (8)
H2	0.319847	0.772106	−0.033323	0.026*
C20	0.8274 (4)	0.7603 (4)	0.04025 (17)	0.0175 (7)
H20	0.767028	0.818420	0.025928	0.021*
C17	0.9999 (5)	0.5935 (4)	0.08156 (18)	0.0215 (8)
H17	1.057912	0.534030	0.096134	0.026*
C5	0.4765 (4)	0.9423 (4)	0.10083 (16)	0.0152 (7)

C7	0.5236 (4)	1.1185 (4)	0.17918 (17)	0.0185 (8)
H7	0.455457	1.165969	0.161648	0.022*
C6	0.5475 (4)	1.0002 (4)	0.15501 (16)	0.0162 (7)
C11	0.7482 (4)	0.6497 (4)	0.22631 (17)	0.0189 (8)
H11	0.688936	0.702667	0.242198	0.023*
C12	0.7986 (5)	0.5507 (4)	0.25202 (17)	0.0200 (8)
H12	0.777478	0.537798	0.285559	0.024*
C15	0.8624 (4)	0.5978 (4)	0.15622 (16)	0.0157 (7)
C8	0.6014 (5)	1.1659 (4)	0.22958 (17)	0.0206 (8)
H8	0.588245	1.247440	0.246647	0.025*
C19	0.9357 (5)	0.7250 (4)	0.01437 (17)	0.0208 (8)
H19	0.948827	0.757597	−0.017295	0.025*
C9	0.6985 (5)	1.0938 (4)	0.25498 (18)	0.0211 (8)
H9	0.750625	1.123962	0.289801	0.025*
C3	0.2968 (4)	0.9182 (4)	0.02197 (17)	0.0207 (8)
H3	0.214765	0.944598	0.001826	0.025*
C16	0.8910 (4)	0.6331 (4)	0.10567 (16)	0.0158 (7)
C1	0.4762 (4)	0.7779 (4)	0.03212 (16)	0.0182 (7)
H1	0.516609	0.705646	0.018558	0.022*
C14	0.9133 (4)	0.4946 (4)	0.17934 (17)	0.0197 (8)
H14	0.969857	0.440928	0.162279	0.024*
C4	0.3562 (4)	0.9825 (4)	0.07255 (17)	0.0184 (8)
H4	0.315036	1.052700	0.087389	0.022*
C18	1.0233 (5)	0.6418 (4)	0.03578 (18)	0.0230 (8)
H18	1.099428	0.617504	0.019383	0.028*
C10	0.7175 (4)	0.9771 (4)	0.22842 (16)	0.0179 (7)
H10	0.785232	0.928262	0.245294	0.021*
C13	0.8803 (5)	0.4712 (4)	0.22762 (18)	0.0216 (8)
H13	0.913687	0.400990	0.243799	0.026*
Ta3	−0.00635 (2)	0.33576 (2)	0.38898 (2)	0.02034 (4)
Ta4	0.63142 (2)	−0.13811 (2)	0.36861 (2)	0.02023 (4)
Cu2	0.29152 (6)	0.10318 (5)	0.36059 (2)	0.01799 (10)
F21	0.8047 (3)	−0.0728 (3)	0.34984 (13)	0.0329 (7)
F13	0.0337 (3)	0.1905 (3)	0.34529 (12)	0.0312 (6)
F23	0.5569 (3)	−0.2131 (3)	0.29738 (11)	0.0307 (6)
F16	−0.0387 (3)	0.4811 (3)	0.43312 (13)	0.0359 (7)
F24	0.4541 (3)	−0.2063 (4)	0.38472 (13)	0.0458 (9)
F15	−0.1820 (3)	0.3384 (3)	0.34261 (12)	0.0359 (7)
F19	0.5514 (3)	0.0146 (3)	0.35417 (13)	0.0383 (7)
F22	0.7064 (3)	−0.2934 (3)	0.38108 (16)	0.0460 (9)
F14	−0.0971 (4)	0.2243 (3)	0.42789 (14)	0.0484 (9)
F20	0.6966 (4)	−0.0686 (4)	0.44044 (13)	0.0504 (9)
N7	0.1943 (4)	−0.0253 (3)	0.39661 (14)	0.0170 (6)
F17	0.0823 (4)	0.4475 (3)	0.34739 (15)	0.0440 (8)
N5	0.3281 (4)	0.2525 (3)	0.32378 (14)	0.0182 (7)
N6	0.4368 (4)	0.2126 (3)	0.41895 (14)	0.0181 (7)
N8	0.2405 (4)	−0.0415 (3)	0.29996 (15)	0.0191 (7)
F18	0.1739 (4)	0.3349 (4)	0.43259 (17)	0.0627 (12)

C39	0.2640 (5)	−0.1563 (4)	0.21782 (18)	0.0218 (8)
H39	0.291350	−0.154459	0.184489	0.026*
C26	0.4974 (4)	0.3223 (4)	0.40414 (17)	0.0178 (7)
C23	0.3995 (5)	0.4718 (4)	0.2798 (2)	0.0259 (9)
H23	0.426235	0.545695	0.264082	0.031*
C35	0.1492 (4)	−0.1430 (4)	0.36712 (16)	0.0168 (7)
C33	0.0475 (5)	−0.2200 (4)	0.43722 (18)	0.0221 (8)
H33	−0.002722	−0.287185	0.451181	0.027*
C37	0.1677 (4)	−0.2708 (4)	0.28085 (17)	0.0199 (8)
H37	0.129683	−0.348965	0.291495	0.024*
C22	0.2878 (5)	0.3774 (4)	0.25324 (18)	0.0233 (8)
H22	0.234903	0.387033	0.219656	0.028*
C31	0.1648 (4)	−0.0038 (4)	0.44524 (17)	0.0202 (8)
H31	0.192692	0.080082	0.465036	0.024*
C34	0.0740 (5)	−0.2408 (4)	0.38662 (18)	0.0212 (8)
H34	0.040589	−0.322079	0.365254	0.025*
C27	0.6082 (5)	0.4046 (5)	0.43749 (19)	0.0254 (9)
H27	0.649078	0.480936	0.426353	0.030*
C32	0.0950 (5)	−0.1001 (4)	0.46741 (18)	0.0217 (8)
H32	0.079950	−0.084253	0.502625	0.026*
C36	0.1841 (4)	−0.1539 (4)	0.31391 (16)	0.0166 (7)
C29	0.5970 (5)	0.2631 (5)	0.50230 (19)	0.0272 (9)
H29	0.629406	0.241474	0.536481	0.033*
C21	0.2552 (5)	0.2689 (4)	0.27675 (17)	0.0214 (8)
H21	0.178536	0.204241	0.258864	0.026*
C25	0.4332 (4)	0.3463 (4)	0.35056 (17)	0.0180 (7)
C24	0.4716 (5)	0.4571 (4)	0.32964 (18)	0.0226 (8)
H24	0.545932	0.522120	0.348967	0.027*
C38	0.2078 (5)	−0.2715 (4)	0.23199 (19)	0.0232 (9)
H38	0.196865	−0.350143	0.208612	0.028*
C30	0.4876 (5)	0.1833 (4)	0.46724 (17)	0.0215 (8)
H30	0.447016	0.105492	0.477449	0.026*
C40	0.2796 (5)	−0.0435 (4)	0.25308 (17)	0.0215 (8)
H40	0.319631	0.035248	0.243508	0.026*
C28	0.6592 (5)	0.3750 (5)	0.4873 (2)	0.0293 (10)
H28	0.735536	0.430406	0.510793	0.035*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ta2	0.01384 (7)	0.01637 (7)	0.01688 (8)	0.00172 (5)	0.00301 (6)	0.00224 (6)
Ta1	0.01627 (8)	0.01625 (8)	0.02005 (8)	0.00161 (6)	0.00173 (6)	0.00487 (6)
Cu1	0.0163 (2)	0.0154 (2)	0.0156 (2)	0.00803 (17)	0.00351 (17)	0.00329 (17)
F9	0.0252 (13)	0.0316 (14)	0.0196 (13)	0.0051 (11)	0.0082 (10)	0.0003 (10)
F5	0.0206 (12)	0.0359 (15)	0.0268 (14)	0.0074 (11)	0.0059 (10)	0.0120 (12)
F8	0.0158 (11)	0.0372 (15)	0.0237 (13)	−0.0007 (10)	0.0022 (10)	0.0056 (11)
F12	0.0263 (13)	0.0245 (13)	0.0211 (13)	0.0048 (10)	0.0066 (10)	−0.0008 (10)
F11	0.0153 (11)	0.0350 (15)	0.0263 (14)	0.0025 (10)	0.0027 (10)	−0.0012 (11)

F3	0.0234 (12)	0.0226 (12)	0.0267 (14)	0.0041 (10)	−0.0023 (10)	0.0076 (10)
F7	0.0364 (15)	0.0221 (13)	0.0290 (15)	0.0037 (11)	0.0015 (12)	0.0091 (11)
F4	0.0407 (16)	0.0173 (12)	0.0287 (15)	0.0020 (11)	−0.0023 (12)	0.0000 (11)
F10	0.0352 (15)	0.0184 (12)	0.0280 (14)	0.0070 (10)	0.0140 (11)	0.0069 (10)
F2	0.0247 (14)	0.0439 (17)	0.0319 (16)	0.0030 (12)	0.0093 (12)	0.0062 (13)
F6	0.0278 (13)	0.0303 (14)	0.0227 (13)	0.0026 (11)	0.0000 (11)	0.0117 (11)
F1	0.0296 (14)	0.0183 (12)	0.0300 (15)	0.0009 (10)	0.0004 (11)	0.0029 (10)
N3	0.0158 (15)	0.0143 (14)	0.0187 (16)	0.0053 (12)	0.0041 (12)	0.0016 (12)
N1	0.0146 (14)	0.0137 (14)	0.0202 (17)	0.0051 (11)	0.0038 (12)	0.0038 (12)
N4	0.0160 (15)	0.0129 (14)	0.0174 (16)	0.0022 (11)	0.0033 (12)	0.0038 (12)
N2	0.0160 (15)	0.0150 (14)	0.0175 (16)	0.0050 (12)	0.0046 (12)	0.0029 (12)
C2	0.0221 (19)	0.0216 (19)	0.020 (2)	0.0054 (15)	−0.0001 (16)	0.0030 (16)
C20	0.0166 (17)	0.0168 (17)	0.0206 (19)	0.0036 (14)	0.0042 (15)	0.0069 (14)
C17	0.0194 (19)	0.022 (2)	0.024 (2)	0.0082 (15)	0.0056 (16)	0.0004 (16)
C5	0.0154 (16)	0.0151 (16)	0.0179 (18)	0.0046 (13)	0.0060 (14)	0.0066 (14)
C7	0.0164 (17)	0.0166 (17)	0.024 (2)	0.0054 (14)	0.0058 (15)	0.0023 (15)
C6	0.0149 (17)	0.0159 (17)	0.0205 (19)	0.0054 (13)	0.0062 (14)	0.0061 (14)
C11	0.0187 (18)	0.0192 (18)	0.0190 (19)	0.0046 (14)	0.0036 (15)	0.0022 (15)
C12	0.0231 (19)	0.0213 (19)	0.0171 (19)	0.0032 (15)	0.0043 (15)	0.0082 (15)
C15	0.0139 (16)	0.0158 (17)	0.0175 (18)	0.0043 (13)	0.0022 (14)	0.0016 (14)
C8	0.0221 (19)	0.0179 (18)	0.022 (2)	0.0032 (15)	0.0071 (16)	−0.0005 (15)
C19	0.0218 (19)	0.0219 (19)	0.020 (2)	0.0021 (15)	0.0085 (16)	0.0030 (15)
C9	0.0214 (19)	0.0197 (19)	0.021 (2)	0.0008 (15)	0.0043 (16)	−0.0010 (15)
C3	0.0170 (18)	0.024 (2)	0.021 (2)	0.0066 (15)	0.0005 (15)	0.0056 (16)
C16	0.0163 (17)	0.0135 (16)	0.0176 (18)	0.0029 (13)	0.0032 (14)	0.0013 (13)
C1	0.0207 (18)	0.0179 (18)	0.0177 (19)	0.0067 (15)	0.0046 (15)	0.0032 (14)
C14	0.0188 (18)	0.0176 (18)	0.023 (2)	0.0048 (14)	0.0033 (15)	0.0016 (15)
C4	0.0164 (17)	0.0169 (17)	0.024 (2)	0.0069 (14)	0.0039 (15)	0.0047 (15)
C18	0.021 (2)	0.025 (2)	0.025 (2)	0.0069 (16)	0.0092 (17)	0.0003 (17)
C10	0.0192 (18)	0.0190 (18)	0.0163 (18)	0.0045 (14)	0.0037 (14)	0.0033 (14)
C13	0.023 (2)	0.0180 (18)	0.023 (2)	0.0063 (15)	−0.0007 (16)	0.0056 (15)
Ta3	0.02110 (8)	0.01596 (8)	0.02421 (9)	0.00380 (6)	0.00382 (6)	0.00350 (6)
Ta4	0.01788 (8)	0.02380 (9)	0.01855 (9)	0.00452 (6)	0.00136 (6)	0.00287 (6)
Cu2	0.0231 (2)	0.0138 (2)	0.0162 (2)	−0.00050 (18)	0.00276 (19)	0.00333 (17)
F21	0.0188 (13)	0.0342 (15)	0.0464 (18)	0.0008 (11)	0.0027 (12)	0.0167 (14)
F13	0.0352 (15)	0.0216 (13)	0.0429 (18)	0.0083 (11)	0.0209 (13)	0.0048 (12)
F23	0.0284 (14)	0.0391 (16)	0.0215 (14)	0.0037 (12)	0.0046 (11)	−0.0073 (12)
F16	0.0457 (18)	0.0243 (14)	0.0370 (17)	0.0067 (13)	0.0116 (14)	−0.0048 (12)
F24	0.0234 (14)	0.084 (3)	0.0337 (18)	0.0028 (16)	0.0096 (13)	0.0226 (17)
F15	0.0379 (16)	0.0344 (16)	0.0317 (16)	0.0131 (13)	−0.0044 (13)	−0.0014 (13)
F19	0.0375 (16)	0.0310 (16)	0.0461 (19)	0.0211 (13)	0.0008 (14)	−0.0011 (14)
F22	0.0273 (15)	0.0263 (15)	0.078 (3)	0.0024 (12)	−0.0137 (16)	0.0199 (16)
F14	0.078 (3)	0.0344 (17)	0.049 (2)	0.0158 (17)	0.0395 (19)	0.0197 (15)
F20	0.065 (2)	0.057 (2)	0.0195 (15)	−0.0035 (18)	−0.0066 (15)	−0.0008 (14)
N7	0.0184 (15)	0.0156 (15)	0.0169 (16)	0.0031 (12)	0.0034 (12)	0.0013 (12)
F17	0.057 (2)	0.0232 (14)	0.059 (2)	−0.0018 (14)	0.0350 (18)	0.0055 (14)
N5	0.0195 (16)	0.0171 (15)	0.0180 (16)	0.0004 (12)	0.0040 (13)	0.0043 (12)
N6	0.0187 (16)	0.0181 (16)	0.0180 (16)	0.0049 (13)	0.0036 (13)	0.0018 (13)

N8	0.0195 (16)	0.0139 (15)	0.0237 (18)	0.0016 (12)	0.0044 (13)	0.0026 (13)
F18	0.041 (2)	0.071 (3)	0.064 (3)	0.0237 (19)	−0.0188 (18)	−0.012 (2)
C39	0.0202 (19)	0.025 (2)	0.019 (2)	0.0033 (16)	0.0034 (15)	−0.0007 (16)
C26	0.0147 (17)	0.0155 (17)	0.023 (2)	0.0020 (13)	0.0037 (15)	0.0021 (14)
C23	0.030 (2)	0.020 (2)	0.031 (2)	0.0057 (17)	0.0095 (19)	0.0116 (17)
C35	0.0135 (16)	0.0165 (17)	0.0200 (19)	0.0014 (13)	0.0018 (14)	0.0037 (14)
C33	0.0183 (18)	0.022 (2)	0.028 (2)	0.0023 (15)	0.0066 (16)	0.0101 (17)
C37	0.0213 (19)	0.0141 (17)	0.023 (2)	0.0011 (14)	0.0027 (16)	0.0014 (15)
C22	0.026 (2)	0.024 (2)	0.022 (2)	0.0052 (17)	0.0053 (17)	0.0082 (16)
C31	0.0211 (19)	0.0186 (18)	0.022 (2)	0.0045 (15)	0.0045 (16)	0.0049 (15)
C34	0.0204 (19)	0.0154 (18)	0.028 (2)	0.0007 (15)	0.0048 (16)	0.0053 (16)
C27	0.020 (2)	0.027 (2)	0.027 (2)	−0.0026 (16)	0.0034 (17)	0.0016 (18)
C32	0.0207 (19)	0.023 (2)	0.025 (2)	0.0065 (16)	0.0071 (16)	0.0086 (16)
C36	0.0125 (16)	0.0164 (17)	0.0197 (19)	0.0006 (13)	0.0008 (14)	0.0032 (14)
C29	0.020 (2)	0.039 (3)	0.022 (2)	0.0058 (18)	0.0002 (17)	0.0043 (19)
C21	0.0223 (19)	0.0221 (19)	0.020 (2)	0.0009 (16)	0.0050 (16)	0.0050 (16)
C25	0.0167 (17)	0.0158 (17)	0.022 (2)	0.0039 (14)	0.0047 (15)	0.0036 (15)
C24	0.024 (2)	0.0172 (18)	0.026 (2)	−0.0018 (15)	0.0049 (17)	0.0045 (16)
C38	0.0195 (19)	0.021 (2)	0.027 (2)	0.0038 (15)	0.0021 (16)	−0.0019 (16)
C30	0.0205 (19)	0.025 (2)	0.019 (2)	0.0028 (16)	0.0031 (15)	0.0041 (16)
C40	0.026 (2)	0.0195 (19)	0.019 (2)	0.0031 (16)	0.0027 (16)	0.0043 (15)
C28	0.022 (2)	0.036 (3)	0.026 (2)	−0.0040 (18)	0.0003 (18)	0.0021 (19)

Geometric parameters (Å, °)

Ta2—F9	1.902 (3)	Ta3—F13	1.910 (3)
Ta2—F8	1.893 (2)	Ta3—F16	1.889 (3)
Ta2—F12	1.894 (3)	Ta3—F15	1.887 (3)
Ta2—F11	1.896 (2)	Ta3—F14	1.870 (3)
Ta2—F7	1.897 (3)	Ta3—F17	1.912 (3)
Ta2—F10	1.898 (3)	Ta3—F18	1.886 (3)
Ta1—F5	1.899 (3)	Ta4—F21	1.883 (3)
Ta1—F3	1.894 (3)	Ta4—F23	1.901 (3)
Ta1—F4	1.888 (3)	Ta4—F24	1.896 (3)
Ta1—F2	1.892 (3)	Ta4—F19	1.903 (3)
Ta1—F6	1.893 (3)	Ta4—F22	1.895 (3)
Ta1—F1	1.913 (3)	Ta4—F20	1.889 (3)
Cu1—F7	2.987 (3)	Cu2—F13	2.706 (3)
Cu1—F1	2.537 (3)	Cu2—F19	2.775 (3)
Cu1—N3	1.982 (3)	Cu2—N7	1.968 (3)
Cu1—N1	1.972 (3)	Cu2—N5	1.960 (3)
Cu1—N4	1.964 (3)	Cu2—N6	2.005 (4)
Cu1—N2	1.977 (3)	Cu2—N8	2.006 (4)
N3—C11	1.347 (5)	N7—C35	1.356 (5)
N3—C15	1.348 (5)	N7—C31	1.342 (5)
N1—C5	1.354 (5)	N5—C21	1.335 (6)
N1—C1	1.344 (5)	N5—C25	1.351 (5)
N4—C20	1.332 (5)	N6—C26	1.356 (5)

N4—C16	1.353 (5)	N6—C30	1.346 (6)
N2—C6	1.362 (5)	N8—C36	1.356 (5)
N2—C10	1.337 (5)	N8—C40	1.335 (6)
C2—H2	0.9500	C39—H39	0.9500
C2—C3	1.382 (6)	C39—C38	1.383 (6)
C2—C1	1.390 (6)	C39—C40	1.386 (6)
C20—H20	0.9500	C26—C27	1.379 (6)
C20—C19	1.392 (6)	C26—C25	1.481 (6)
C17—H17	0.9500	C23—H23	0.9500
C17—C16	1.385 (6)	C23—C22	1.389 (7)
C17—C18	1.390 (6)	C23—C24	1.388 (7)
C5—C6	1.475 (6)	C35—C34	1.382 (6)
C5—C4	1.387 (5)	C35—C36	1.474 (6)
C7—H7	0.9500	C33—H33	0.9500
C7—C6	1.388 (5)	C33—C34	1.380 (6)
C7—C8	1.389 (6)	C33—C32	1.385 (6)
C11—H11	0.9500	C37—H37	0.9500
C11—C12	1.388 (6)	C37—C36	1.390 (6)
C12—H12	0.9500	C37—C38	1.389 (6)
C12—C13	1.383 (6)	C22—H22	0.9500
C15—C16	1.468 (6)	C22—C21	1.385 (6)
C15—C14	1.395 (6)	C31—H31	0.9500
C8—H8	0.9500	C31—C32	1.385 (6)
C8—C9	1.390 (6)	C34—H34	0.9500
C19—H19	0.9500	C27—H27	0.9500
C19—C18	1.375 (6)	C27—C28	1.384 (7)
C9—H9	0.9500	C32—H32	0.9500
C9—C10	1.382 (6)	C29—H29	0.9500
C3—H3	0.9500	C29—C30	1.380 (6)
C3—C4	1.394 (6)	C29—C28	1.383 (7)
C1—H1	0.9500	C21—H21	0.9500
C14—H14	0.9500	C25—C24	1.381 (6)
C14—C13	1.389 (6)	C24—H24	0.9500
C4—H4	0.9500	C38—H38	0.9500
C18—H18	0.9500	C30—H30	0.9500
C10—H10	0.9500	C40—H40	0.9500
C13—H13	0.9500	C28—H28	0.9500
F8—Ta2—F9	92.66 (12)	F13—Ta3—F17	89.01 (13)
F8—Ta2—F12	89.58 (12)	F16—Ta3—F13	177.92 (14)
F8—Ta2—F11	177.33 (12)	F16—Ta3—F17	90.17 (14)
F8—Ta2—F7	87.35 (12)	F15—Ta3—F13	91.30 (13)
F8—Ta2—F10	88.94 (12)	F15—Ta3—F16	90.58 (14)
F12—Ta2—F9	176.38 (11)	F15—Ta3—F17	87.30 (16)
F12—Ta2—F11	88.98 (12)	F14—Ta3—F13	90.20 (13)
F12—Ta2—F7	92.89 (12)	F14—Ta3—F16	90.66 (14)
F12—Ta2—F10	88.43 (11)	F14—Ta3—F15	91.22 (17)
F11—Ta2—F9	88.88 (11)	F14—Ta3—F17	178.31 (17)

F11—Ta2—F7	90.47 (12)	F14—Ta3—F18	91.3 (2)
F11—Ta2—F10	93.28 (12)	F18—Ta3—F13	87.43 (16)
F7—Ta2—F9	90.05 (12)	F18—Ta3—F16	90.66 (16)
F7—Ta2—F10	176.05 (12)	F18—Ta3—F15	177.17 (18)
F10—Ta2—F9	88.78 (12)	F18—Ta3—F17	90.2 (2)
F5—Ta1—F1	87.61 (12)	F21—Ta4—F23	90.32 (13)
F3—Ta1—F5	89.44 (12)	F21—Ta4—F24	177.79 (14)
F3—Ta1—F1	89.06 (11)	F21—Ta4—F19	90.96 (14)
F4—Ta1—F5	92.10 (13)	F21—Ta4—F22	89.84 (14)
F4—Ta1—F3	90.64 (12)	F21—Ta4—F20	92.80 (16)
F4—Ta1—F2	91.12 (14)	F23—Ta4—F19	89.22 (14)
F4—Ta1—F6	90.26 (12)	F24—Ta4—F23	87.48 (14)
F4—Ta1—F1	179.59 (13)	F24—Ta4—F19	88.86 (16)
F2—Ta1—F5	176.73 (13)	F22—Ta4—F23	89.03 (15)
F2—Ta1—F3	91.08 (13)	F22—Ta4—F24	90.27 (16)
F2—Ta1—F6	89.72 (13)	F22—Ta4—F19	178.08 (14)
F2—Ta1—F1	89.17 (13)	F20—Ta4—F23	176.84 (15)
F6—Ta1—F5	89.71 (12)	F20—Ta4—F24	89.40 (16)
F6—Ta1—F3	178.79 (12)	F20—Ta4—F19	91.22 (16)
F6—Ta1—F1	90.04 (12)	F20—Ta4—F22	90.48 (17)
F1—Cu1—F7	161.46 (9)	F13—Cu2—F19	168.21 (10)
N3—Cu1—F7	83.17 (11)	N7—Cu2—F13	83.91 (12)
N3—Cu1—F1	81.03 (12)	N7—Cu2—F19	103.51 (12)
N1—Cu1—F7	118.40 (11)	N7—Cu2—N6	103.87 (14)
N1—Cu1—F1	78.18 (12)	N7—Cu2—N8	82.29 (14)
N1—Cu1—N3	158.21 (14)	N5—Cu2—F13	77.43 (12)
N1—Cu1—N2	83.13 (14)	N5—Cu2—F19	95.18 (13)
N4—Cu1—F7	70.99 (11)	N5—Cu2—N7	161.27 (15)
N4—Cu1—F1	116.26 (12)	N5—Cu2—N6	82.25 (15)
N4—Cu1—N3	82.84 (14)	N5—Cu2—N8	101.20 (15)
N4—Cu1—N1	100.59 (14)	N6—Cu2—F13	113.10 (12)
N4—Cu1—N2	150.27 (14)	N6—Cu2—F19	74.40 (12)
N2—Cu1—F7	81.24 (11)	N6—Cu2—N8	150.51 (14)
N2—Cu1—F1	93.43 (12)	N8—Cu2—F13	96.12 (12)
N2—Cu1—N3	104.65 (14)	N8—Cu2—F19	76.12 (12)
Ta2—F7—Cu1	114.17 (12)	Ta3—F13—Cu2	122.63 (14)
Ta1—F1—Cu1	125.65 (14)	Ta4—F19—Cu2	135.07 (17)
C11—N3—Cu1	126.4 (3)	C35—N7—Cu2	114.6 (3)
C11—N3—C15	119.5 (3)	C31—N7—Cu2	125.9 (3)
C15—N3—Cu1	112.8 (3)	C31—N7—C35	119.4 (4)
C5—N1—Cu1	113.7 (3)	C21—N5—Cu2	125.5 (3)
C1—N1—Cu1	126.0 (3)	C21—N5—C25	119.5 (4)
C1—N1—C5	119.8 (3)	C25—N5—Cu2	115.0 (3)
C20—N4—Cu1	125.2 (3)	C26—N6—Cu2	113.1 (3)
C20—N4—C16	119.9 (3)	C30—N6—Cu2	127.7 (3)
C16—N4—Cu1	113.6 (3)	C30—N6—C26	118.8 (4)
C6—N2—Cu1	112.9 (3)	C36—N8—Cu2	112.8 (3)
C10—N2—Cu1	126.5 (3)	C40—N8—Cu2	127.0 (3)

C10—N2—C6	119.5 (3)	C40—N8—C36	118.9 (4)
C3—C2—H2	120.5	C38—C39—H39	120.6
C3—C2—C1	118.9 (4)	C38—C39—C40	118.9 (4)
C1—C2—H2	120.5	C40—C39—H39	120.6
N4—C20—H20	118.9	N6—C26—C27	121.6 (4)
N4—C20—C19	122.2 (4)	N6—C26—C25	114.7 (3)
C19—C20—H20	118.9	C27—C26—C25	123.7 (4)
C16—C17—H17	120.4	C22—C23—H23	120.3
C16—C17—C18	119.3 (4)	C24—C23—H23	120.3
C18—C17—H17	120.4	C24—C23—C22	119.4 (4)
N1—C5—C6	114.6 (3)	N7—C35—C34	120.8 (4)
N1—C5—C4	121.3 (4)	N7—C35—C36	114.5 (3)
C4—C5—C6	124.1 (4)	C34—C35—C36	124.7 (4)
C6—C7—H7	120.7	C34—C33—H33	120.4
C6—C7—C8	118.5 (4)	C34—C33—C32	119.2 (4)
C8—C7—H7	120.7	C32—C33—H33	120.4
N2—C6—C5	114.9 (3)	C36—C37—H37	120.5
N2—C6—C7	121.4 (4)	C38—C37—H37	120.5
C7—C6—C5	123.7 (4)	C38—C37—C36	118.9 (4)
N3—C11—H11	118.9	C23—C22—H22	120.7
N3—C11—C12	122.3 (4)	C21—C22—C23	118.6 (4)
C12—C11—H11	118.9	C21—C22—H22	120.7
C11—C12—H12	120.8	N7—C31—H31	119.0
C13—C12—C11	118.4 (4)	N7—C31—C32	121.9 (4)
C13—C12—H12	120.8	C32—C31—H31	119.0
N3—C15—C16	114.7 (3)	C35—C34—H34	120.1
N3—C15—C14	121.0 (4)	C33—C34—C35	119.8 (4)
C14—C15—C16	124.3 (4)	C33—C34—H34	120.1
C7—C8—H8	120.1	C26—C27—H27	120.3
C7—C8—C9	119.9 (4)	C26—C27—C28	119.5 (4)
C9—C8—H8	120.1	C28—C27—H27	120.3
C20—C19—H19	120.8	C33—C32—H32	120.6
C18—C19—C20	118.4 (4)	C31—C32—C33	118.7 (4)
C18—C19—H19	120.8	C31—C32—H32	120.6
C8—C9—H9	120.8	N8—C36—C35	115.0 (3)
C10—C9—C8	118.5 (4)	N8—C36—C37	121.6 (4)
C10—C9—H9	120.8	C37—C36—C35	123.3 (4)
C2—C3—H3	120.2	C30—C29—H29	120.2
C2—C3—C4	119.5 (4)	C30—C29—C28	119.5 (4)
C4—C3—H3	120.2	C28—C29—H29	120.2
N4—C16—C17	120.7 (4)	N5—C21—C22	122.0 (4)
N4—C16—C15	114.5 (3)	N5—C21—H21	119.0
C17—C16—C15	124.7 (4)	C22—C21—H21	119.0
N1—C1—C2	121.6 (4)	N5—C25—C26	114.5 (3)
N1—C1—H1	119.2	N5—C25—C24	121.7 (4)
C2—C1—H1	119.2	C24—C25—C26	123.8 (4)
C15—C14—H14	120.4	C23—C24—H24	120.6
C13—C14—C15	119.1 (4)	C25—C24—C23	118.7 (4)

C13—C14—H14	120.4	C25—C24—H24	120.6
C5—C4—C3	118.9 (4)	C39—C38—C37	119.2 (4)
C5—C4—H4	120.6	C39—C38—H38	120.4
C3—C4—H4	120.6	C37—C38—H38	120.4
C17—C18—H18	120.2	N6—C30—C29	121.8 (4)
C19—C18—C17	119.6 (4)	N6—C30—H30	119.1
C19—C18—H18	120.2	C29—C30—H30	119.1
N2—C10—C9	122.3 (4)	N8—C40—C39	122.5 (4)
N2—C10—H10	118.9	N8—C40—H40	118.8
C9—C10—H10	118.9	C39—C40—H40	118.8
C12—C13—C14	119.7 (4)	C27—C28—H28	120.6
C12—C13—H13	120.2	C29—C28—C27	118.8 (4)
C14—C13—H13	120.2	C29—C28—H28	120.6

Tris(2,2'-bipyridine- κ^2N,N')copper(II) bis[hexafluoridotantalate(V)] (III)

Crystal data

[Cu(C₁₀H₈N₂)₃][TaF₆]₂

$M_r = 1121.99$

Trigonal, $P3_2$

$a = 10.5172$ (10) Å

$c = 26.288$ (2) Å

$V = 2518.2$ (5) Å³

$Z = 3$

$F(000) = 1587$

$D_x = 2.220$ Mg m⁻³

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

Cell parameters from 9702 reflections

$\theta = 2.2$ – 32.5°

$\mu = 7.23$ mm⁻¹

$T = 100$ K

Block, blue

$0.22 \times 0.16 \times 0.12$ mm

Data collection

Bruker Kappa APEX CCD area detector
diffractometer

Radiation source: sealed tube

Triumph monochromator

Detector resolution: 8 pixels mm⁻¹

ω and ϕ scans

Absorption correction: multi-scan

(SADABS; Bruker, 2016)

$T_{\min} = 0.559$, $T_{\max} = 0.746$

148130 measured reflections

12260 independent reflections

12121 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$

$\theta_{\max} = 32.7^\circ$, $\theta_{\min} = 1.6^\circ$

$h = -15 \rightarrow 15$

$k = -15 \rightarrow 15$

$l = -38 \rightarrow 39$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.031$

$S = 1.03$

12260 reflections

462 parameters

1 restraint

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0106P)^2 + 0.1438P]$

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

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.96$ e Å⁻³

$\Delta\rho_{\min} = -0.85$ e Å⁻³

Extinction correction: SHELXL-2018/3

(Sheldrick 2015b),

$F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00031 (3)

Absolute structure: Flack x determined using

5861 quotients $[(F^+) - (F^-)] / [(F^+) + (F^-)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: 0.5036 (7)

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.

Refinement. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ta2	0.00684 (3)	−0.03219 (2)	0.32198 (2)	0.01774 (4)
Ta1	0.70686 (2)	1.36139 (2)	0.47151 (2)	0.01986 (4)
Cu1	0.32411 (6)	0.64362 (5)	0.57036 (2)	0.01228 (8)
F2	0.5183 (3)	1.2403 (5)	0.44310 (13)	0.0633 (12)
F4	0.7724 (4)	1.2402 (3)	0.44119 (10)	0.0408 (7)
C17	−0.0981 (5)	0.5633 (6)	0.6138 (2)	0.0188 (9)
H17	−0.153152	0.611150	0.608263	0.023*
F8	−0.1759 (3)	−0.0847 (3)	0.35333 (9)	0.0300 (6)
N4	0.1166 (4)	0.5474 (4)	0.59777 (12)	0.0126 (6)
F5	0.9006 (3)	1.4788 (3)	0.49516 (10)	0.0347 (6)
F12	0.0952 (3)	0.0141 (3)	0.38681 (9)	0.0402 (7)
F6	0.6515 (4)	1.2435 (3)	0.53047 (10)	0.0494 (9)
C16	0.0368 (5)	0.6141 (5)	0.59049 (14)	0.0130 (8)
C18	−0.1519 (4)	0.4417 (5)	0.64542 (14)	0.0220 (7)
H18	−0.243559	0.406714	0.662085	0.026*
F9	−0.0912 (3)	−0.0756 (3)	0.25849 (8)	0.0268 (5)
N3	0.2459 (3)	0.8080 (3)	0.54816 (11)	0.0142 (5)
F3	0.7575 (3)	1.4716 (3)	0.41088 (10)	0.0428 (7)
F10	−0.0341 (3)	−0.2286 (3)	0.32783 (10)	0.0295 (6)
F11	0.1857 (3)	0.0098 (3)	0.29071 (10)	0.0305 (6)
F7	0.0551 (3)	0.1672 (3)	0.31516 (9)	0.0283 (5)
F1	0.6482 (4)	1.4867 (4)	0.50135 (13)	0.0455 (8)
C15	0.1004 (4)	0.7442 (4)	0.55624 (12)	0.0138 (6)
C19	−0.0715 (5)	0.3711 (4)	0.65269 (15)	0.0194 (7)
H19	−0.107200	0.286719	0.673773	0.023*
N2	0.5147 (4)	0.7648 (4)	0.53243 (12)	0.0135 (7)
N5	0.4063 (3)	0.7268 (3)	0.64157 (10)	0.0152 (5)
C9	0.7449 (6)	0.9811 (6)	0.51576 (17)	0.0206 (10)
H9	0.823892	1.071865	0.527435	0.025*
C6	0.5147 (4)	0.7167 (4)	0.48464 (13)	0.0138 (6)
C23	0.5294 (5)	0.8446 (5)	0.73468 (18)	0.0230 (10)
H23	0.573816	0.885667	0.766493	0.028*
C24	0.5230 (4)	0.7175 (5)	0.71745 (14)	0.0216 (8)
H24	0.562435	0.670166	0.737466	0.026*
C10	0.6291 (5)	0.8936 (5)	0.54776 (16)	0.0171 (9)
H10	0.630309	0.925531	0.581658	0.021*
C22	0.4708 (5)	0.9115 (4)	0.70528 (14)	0.0216 (7)
H22	0.471689	0.997549	0.716782	0.026*

C11	0.3105 (5)	0.9276 (4)	0.51831 (14)	0.0180 (7)
H11	0.413500	0.974026	0.512970	0.022*
C21	0.4108 (4)	0.8499 (4)	0.65868 (14)	0.0191 (8)
H21	0.371299	0.895865	0.637984	0.023*
C20	0.0634 (4)	0.4284 (4)	0.62794 (13)	0.0157 (7)
H20	0.119861	0.381628	0.632587	0.019*
N1	0.2704 (3)	0.5298 (3)	0.50323 (10)	0.0130 (5)
C5	0.3856 (4)	0.5755 (4)	0.47127 (12)	0.0135 (6)
C7	0.6286 (4)	0.7992 (4)	0.45095 (14)	0.0205 (8)
H7	0.627957	0.763870	0.417631	0.025*
N6	0.3922 (4)	0.4832 (4)	0.60312 (12)	0.0180 (6)
C26	0.4437 (4)	0.5196 (4)	0.65109 (13)	0.0164 (6)
C8	0.7437 (5)	0.9345 (5)	0.46684 (15)	0.0240 (8)
H8	0.820854	0.994029	0.444011	0.029*
C13	0.0833 (4)	0.9178 (4)	0.50245 (13)	0.0196 (7)
H13	0.027481	0.954984	0.486504	0.023*
C25	0.4586 (4)	0.6591 (4)	0.67064 (13)	0.0150 (6)
C14	0.0144 (4)	0.7946 (4)	0.53329 (13)	0.0179 (7)
H14	−0.088668	0.745881	0.538648	0.022*
C12	0.2327 (4)	0.9860 (4)	0.49499 (14)	0.0185 (7)
H12	0.281469	1.071236	0.474305	0.022*
C27	0.4749 (5)	0.4294 (5)	0.68023 (15)	0.0241 (9)
H27	0.510287	0.456347	0.714018	0.029*
C2	0.1346 (5)	0.3167 (4)	0.45214 (16)	0.0225 (8)
H2	0.045309	0.228062	0.445925	0.027*
C1	0.1471 (4)	0.4030 (4)	0.49352 (14)	0.0174 (7)
H1	0.065657	0.371517	0.515813	0.021*
C30	0.3758 (4)	0.3587 (4)	0.58279 (15)	0.0201 (7)
H30	0.343309	0.335632	0.548553	0.024*
C3	0.2530 (5)	0.3601 (4)	0.41977 (15)	0.0250 (8)
H3	0.247427	0.300756	0.391649	0.030*
C4	0.3810 (5)	0.4932 (4)	0.42942 (14)	0.0218 (8)
H4	0.463614	0.526892	0.407591	0.026*
C28	0.4537 (5)	0.2983 (5)	0.65946 (16)	0.0272 (9)
H28	0.472935	0.234061	0.679147	0.033*
C29	0.4043 (5)	0.2626 (5)	0.60978 (16)	0.0234 (8)
H29	0.390410	0.174533	0.594640	0.028*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ta2	0.01698 (8)	0.01449 (10)	0.01536 (7)	0.00308 (8)	−0.00052 (7)	0.00018 (7)
Ta1	0.01754 (9)	0.01929 (10)	0.01742 (7)	0.00521 (9)	0.00037 (7)	0.00145 (8)
Cu1	0.01235 (18)	0.0136 (2)	0.0094 (2)	0.00535 (17)	0.00046 (17)	−0.00043 (14)
F2	0.0201 (13)	0.077 (3)	0.0550 (18)	−0.0039 (17)	−0.0002 (12)	−0.019 (2)
F4	0.056 (2)	0.0339 (17)	0.0316 (14)	0.0220 (16)	0.0046 (14)	−0.0086 (12)
C17	0.018 (2)	0.019 (2)	0.0220 (19)	0.0108 (17)	0.0047 (18)	−0.0006 (18)
F8	0.0297 (12)	0.0280 (14)	0.0236 (11)	0.0079 (11)	0.0091 (9)	0.0002 (10)

N4	0.0142 (14)	0.0117 (15)	0.0106 (13)	0.0056 (12)	0.0025 (10)	0.0018 (11)
F5	0.0275 (12)	0.0382 (16)	0.0390 (14)	0.0169 (13)	−0.0148 (11)	−0.0190 (13)
F12	0.0493 (17)	0.0341 (15)	0.0229 (12)	0.0100 (14)	−0.0170 (12)	−0.0010 (11)
F6	0.074 (3)	0.0418 (16)	0.0303 (13)	0.0279 (18)	0.0220 (15)	0.0169 (12)
C16	0.0189 (19)	0.0114 (16)	0.0080 (16)	0.0071 (15)	0.0001 (13)	0.0001 (13)
C18	0.0182 (16)	0.0188 (18)	0.0262 (18)	0.0071 (16)	0.0076 (14)	0.0031 (16)
F9	0.0312 (12)	0.0345 (13)	0.0178 (10)	0.0188 (11)	−0.0044 (9)	−0.0056 (10)
N3	0.0130 (13)	0.0128 (14)	0.0144 (13)	0.0045 (11)	−0.0013 (11)	−0.0010 (11)
F3	0.0340 (17)	0.0616 (19)	0.0311 (13)	0.0226 (15)	0.0034 (13)	0.0225 (13)
F10	0.0232 (13)	0.0193 (11)	0.0406 (14)	0.0065 (10)	0.0020 (11)	0.0039 (11)
F11	0.0199 (12)	0.0248 (13)	0.0441 (15)	0.0091 (10)	0.0035 (11)	0.0046 (12)
F7	0.0343 (15)	0.0190 (11)	0.0296 (12)	0.0117 (11)	0.0006 (11)	−0.0009 (9)
F1	0.0452 (19)	0.052 (2)	0.0562 (18)	0.0374 (18)	0.0084 (15)	0.0021 (16)
C15	0.0157 (15)	0.0154 (15)	0.0112 (15)	0.0085 (13)	0.0001 (12)	−0.0002 (12)
C19	0.0216 (18)	0.0149 (16)	0.0203 (18)	0.0081 (15)	0.0078 (15)	0.0069 (14)
N2	0.0127 (14)	0.0116 (14)	0.0140 (14)	0.0045 (12)	−0.0019 (10)	−0.0008 (12)
N5	0.0169 (12)	0.0146 (13)	0.0135 (12)	0.0073 (11)	0.0019 (10)	0.0012 (10)
C9	0.017 (2)	0.018 (2)	0.022 (2)	0.0049 (17)	−0.0038 (17)	−0.0039 (18)
C6	0.0152 (14)	0.0142 (16)	0.0128 (14)	0.0079 (13)	0.0014 (11)	−0.0009 (13)
C23	0.026 (2)	0.025 (2)	0.0129 (19)	0.0091 (16)	−0.0027 (17)	−0.0043 (18)
C24	0.0247 (18)	0.025 (2)	0.0124 (16)	0.0105 (16)	−0.0056 (14)	−0.0019 (14)
C10	0.0132 (17)	0.020 (2)	0.0144 (18)	0.0050 (15)	−0.0033 (14)	−0.0005 (15)
C22	0.0217 (19)	0.0186 (15)	0.0183 (16)	0.0054 (16)	−0.0012 (16)	−0.0064 (13)
C11	0.0213 (18)	0.0138 (16)	0.0163 (18)	0.0070 (14)	0.0013 (14)	−0.0006 (13)
C21	0.025 (2)	0.0173 (15)	0.0147 (15)	0.0105 (15)	0.0009 (14)	−0.0006 (12)
C20	0.0182 (17)	0.0139 (15)	0.0159 (16)	0.0087 (14)	0.0017 (13)	0.0016 (13)
N1	0.0131 (13)	0.0134 (12)	0.0130 (12)	0.0069 (11)	−0.0012 (11)	−0.0007 (9)
C5	0.0149 (16)	0.0146 (16)	0.0107 (13)	0.0071 (12)	−0.0003 (12)	−0.0007 (12)
C7	0.0176 (16)	0.0226 (19)	0.0143 (16)	0.0047 (15)	0.0020 (13)	−0.0016 (14)
N6	0.0201 (16)	0.0217 (15)	0.0157 (14)	0.0129 (13)	0.0011 (12)	−0.0002 (12)
C26	0.0128 (16)	0.0210 (19)	0.0147 (15)	0.0078 (14)	0.0021 (14)	0.0025 (14)
C8	0.0173 (18)	0.023 (2)	0.0217 (19)	0.0022 (16)	0.0042 (14)	0.0046 (16)
C13	0.027 (2)	0.0222 (18)	0.0170 (15)	0.0175 (16)	0.0036 (14)	0.0070 (14)
C25	0.0143 (15)	0.0166 (16)	0.0115 (14)	0.0056 (13)	−0.0006 (12)	0.0000 (12)
C14	0.0193 (17)	0.0213 (18)	0.0181 (17)	0.0137 (15)	0.0038 (14)	0.0025 (14)
C12	0.0248 (19)	0.0169 (17)	0.0134 (17)	0.0102 (15)	0.0014 (15)	0.0042 (14)
C27	0.032 (2)	0.033 (2)	0.0150 (17)	0.022 (2)	−0.0067 (16)	−0.0010 (16)
C2	0.0179 (18)	0.0167 (16)	0.0276 (19)	0.0048 (16)	−0.0019 (16)	−0.0068 (14)
C1	0.0173 (17)	0.0141 (15)	0.0170 (16)	0.0050 (13)	0.0002 (14)	−0.0006 (13)
C30	0.0221 (18)	0.0204 (18)	0.0195 (17)	0.0118 (15)	−0.0023 (15)	−0.0033 (15)
C3	0.030 (2)	0.0204 (18)	0.0198 (18)	0.0088 (17)	−0.0024 (17)	−0.0088 (15)
C4	0.0222 (19)	0.0203 (18)	0.0161 (16)	0.0055 (15)	0.0037 (15)	−0.0032 (14)
C28	0.036 (2)	0.033 (2)	0.0241 (19)	0.025 (2)	−0.0039 (18)	0.0042 (18)
C29	0.027 (2)	0.0218 (19)	0.028 (2)	0.0166 (17)	0.0006 (16)	−0.0019 (16)

Geometric parameters (Å, °)

Ta2—F8	1.901 (2)	C23—C24	1.381 (7)
Ta2—F12	1.885 (2)	C23—C22	1.381 (6)
Ta2—F9	1.894 (2)	C24—H24	0.9500
Ta2—F10	1.893 (3)	C24—C25	1.391 (5)
Ta2—F11	1.892 (3)	C10—H10	0.9500
Ta2—F7	1.903 (2)	C22—H22	0.9500
Ta1—F2	1.894 (3)	C22—C21	1.382 (5)
Ta1—F4	1.901 (3)	C11—H11	0.9500
Ta1—F5	1.883 (2)	C11—C12	1.388 (5)
Ta1—F6	1.886 (3)	C21—H21	0.9500
Ta1—F3	1.884 (2)	C20—H20	0.9500
Ta1—F1	1.883 (3)	N1—C5	1.350 (4)
Cu1—N4	2.024 (3)	N1—C1	1.341 (5)
Cu1—N3	2.330 (3)	C5—C4	1.385 (5)
Cu1—N2	2.020 (3)	C7—H7	0.9500
Cu1—N5	2.064 (3)	C7—C8	1.394 (5)
Cu1—N1	2.047 (3)	N6—C26	1.350 (5)
Cu1—N6	2.305 (3)	N6—C30	1.343 (5)
C17—H17	0.9500	C26—C25	1.487 (5)
C17—C16	1.384 (6)	C26—C27	1.380 (5)
C17—C18	1.386 (6)	C8—H8	0.9500
N4—C16	1.350 (6)	C13—H13	0.9500
N4—C20	1.344 (5)	C13—C14	1.386 (5)
C16—C15	1.488 (5)	C13—C12	1.377 (5)
C18—H18	0.9500	C14—H14	0.9500
C18—C19	1.389 (6)	C12—H12	0.9500
N3—C15	1.346 (5)	C27—H27	0.9500
N3—C11	1.343 (5)	C27—C28	1.393 (6)
C15—C14	1.393 (5)	C2—H2	0.9500
C19—H19	0.9500	C2—C1	1.380 (5)
C19—C20	1.394 (5)	C2—C3	1.384 (6)
N2—C6	1.354 (5)	C1—H1	0.9500
N2—C10	1.348 (6)	C30—H30	0.9500
N5—C21	1.349 (4)	C30—C29	1.385 (5)
N5—C25	1.336 (4)	C3—H3	0.9500
C9—H9	0.9500	C3—C4	1.397 (6)
C9—C10	1.384 (7)	C4—H4	0.9500
C9—C8	1.374 (6)	C28—H28	0.9500
C6—C5	1.469 (5)	C28—C29	1.386 (6)
C6—C7	1.390 (5)	C29—H29	0.9500
C23—H23	0.9500		
F8—Ta2—F7	92.03 (12)	C7—C6—C5	123.4 (3)
F12—Ta2—F8	88.82 (12)	C24—C23—H23	120.3
F12—Ta2—F9	176.22 (13)	C22—C23—H23	120.3
F12—Ta2—F10	91.26 (13)	C22—C23—C24	119.5 (4)

F12—Ta2—F11	91.61 (13)	C23—C24—H24	120.2
F12—Ta2—F7	88.58 (12)	C23—C24—C25	119.7 (4)
F9—Ta2—F8	87.85 (10)	C25—C24—H24	120.2
F9—Ta2—F7	89.75 (11)	N2—C10—C9	122.2 (4)
F10—Ta2—F8	90.12 (12)	N2—C10—H10	118.9
F10—Ta2—F9	90.53 (11)	C9—C10—H10	118.9
F10—Ta2—F7	177.84 (12)	C23—C22—H22	120.9
F11—Ta2—F8	177.08 (12)	C23—C22—C21	118.2 (4)
F11—Ta2—F9	91.81 (11)	C21—C22—H22	120.9
F11—Ta2—F10	86.98 (12)	N3—C11—H11	118.7
F11—Ta2—F7	90.87 (12)	N3—C11—C12	122.6 (4)
F2—Ta1—F4	89.58 (16)	C12—C11—H11	118.7
F5—Ta1—F2	175.49 (14)	N5—C21—C22	122.2 (4)
F5—Ta1—F4	86.68 (13)	N5—C21—H21	118.9
F5—Ta1—F6	92.12 (14)	C22—C21—H21	118.9
F5—Ta1—F3	89.74 (13)	N4—C20—C19	122.5 (4)
F6—Ta1—F2	90.39 (16)	N4—C20—H20	118.7
F6—Ta1—F4	90.02 (13)	C19—C20—H20	118.7
F3—Ta1—F2	87.64 (16)	C5—N1—Cu1	113.1 (2)
F3—Ta1—F4	88.41 (14)	C1—N1—Cu1	126.3 (2)
F3—Ta1—F6	177.48 (15)	C1—N1—C5	119.0 (3)
F1—Ta1—F2	92.03 (18)	N1—C5—C6	115.0 (3)
F1—Ta1—F4	178.14 (16)	N1—C5—C4	121.8 (3)
F1—Ta1—F5	91.67 (14)	C4—C5—C6	123.2 (3)
F1—Ta1—F6	90.91 (14)	C6—C7—H7	120.5
F1—Ta1—F3	90.72 (14)	C6—C7—C8	118.9 (3)
N4—Cu1—N3	76.58 (13)	C8—C7—H7	120.5
N4—Cu1—N5	90.44 (12)	C26—N6—Cu1	111.6 (2)
N4—Cu1—N1	95.81 (13)	C30—N6—Cu1	129.0 (3)
N4—Cu1—N6	98.80 (14)	C30—N6—C26	119.1 (3)
N2—Cu1—N4	166.58 (14)	N6—C26—C25	115.6 (3)
N2—Cu1—N3	90.89 (13)	N6—C26—C27	121.5 (4)
N2—Cu1—N5	96.14 (12)	C27—C26—C25	122.8 (3)
N2—Cu1—N1	80.79 (13)	C9—C8—C7	119.5 (4)
N2—Cu1—N6	94.16 (13)	C9—C8—H8	120.2
N5—Cu1—N3	98.11 (11)	C7—C8—H8	120.2
N5—Cu1—N6	75.75 (12)	C14—C13—H13	120.1
N1—Cu1—N3	96.98 (11)	C12—C13—H13	120.1
N1—Cu1—N5	164.65 (12)	C12—C13—C14	119.8 (3)
N1—Cu1—N6	89.41 (11)	N5—C25—C24	120.7 (4)
N6—Cu1—N3	172.42 (10)	N5—C25—C26	117.4 (3)
C16—C17—H17	120.4	C24—C25—C26	121.9 (3)
C16—C17—C18	119.3 (5)	C15—C14—H14	120.9
C18—C17—H17	120.4	C13—C14—C15	118.3 (4)
C16—N4—Cu1	119.0 (3)	C13—C14—H14	120.9
C20—N4—Cu1	121.2 (3)	C11—C12—H12	120.7
C20—N4—C16	119.3 (3)	C13—C12—C11	118.6 (3)
C17—C16—C15	121.7 (4)	C13—C12—H12	120.7

N4—C16—C17	121.3 (4)	C26—C27—H27	120.4
N4—C16—C15	117.0 (4)	C26—C27—C28	119.1 (4)
C17—C18—H18	120.0	C28—C27—H27	120.4
C17—C18—C19	119.9 (4)	C1—C2—H2	120.2
C19—C18—H18	120.0	C1—C2—C3	119.6 (4)
C15—N3—Cu1	109.0 (2)	C3—C2—H2	120.2
C11—N3—Cu1	129.8 (3)	N1—C1—C2	122.0 (4)
C11—N3—C15	118.4 (3)	N1—C1—H1	119.0
N3—C15—C16	115.5 (3)	C2—C1—H1	119.0
N3—C15—C14	122.3 (3)	N6—C30—H30	118.7
C14—C15—C16	122.2 (4)	N6—C30—C29	122.6 (4)
C18—C19—H19	121.2	C29—C30—H30	118.7
C18—C19—C20	117.7 (3)	C2—C3—H3	120.8
C20—C19—H19	121.2	C2—C3—C4	118.4 (4)
C6—N2—Cu1	114.0 (3)	C4—C3—H3	120.8
C10—N2—Cu1	126.3 (3)	C5—C4—C3	119.1 (4)
C10—N2—C6	119.1 (3)	C5—C4—H4	120.5
C21—N5—Cu1	121.0 (2)	C3—C4—H4	120.5
C25—N5—Cu1	119.3 (2)	C27—C28—H28	120.3
C25—N5—C21	119.7 (3)	C29—C28—C27	119.4 (4)
C10—C9—H9	120.5	C29—C28—H28	120.3
C8—C9—H9	120.5	C30—C29—C28	118.3 (4)
C8—C9—C10	118.9 (5)	C30—C29—H29	120.9
N2—C6—C5	115.3 (3)	C28—C29—H29	120.9
N2—C6—C7	121.3 (3)		

catena-Poly[[diaqua(2,2'-bipyridine- κ^2 N,N')copper(II)]- μ -fluorido-tetrafluoridotin- μ -fluorido] (IV)

Crystal data

[CuSnF₆(C₁₀H₈N₂)(H₂O)₂]

$M_r = 488.45$

Monoclinic, $P2_1/n$

$a = 6.2590$ (2) Å

$b = 9.2167$ (3) Å

$c = 12.1648$ (3) Å

$\beta = 90.734$ (2)°

$V = 701.70$ (4) Å³

$Z = 2$

$F(000) = 470$

$D_x = 2.312$ Mg m⁻³

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

Cell parameters from 9773 reflections

$\theta = 2.2\text{--}37.7^\circ$

$\mu = 3.37$ mm⁻¹

$T = 100$ K

Block, blue

$0.20 \times 0.13 \times 0.12$ mm

Data collection

Rigaku Oxford Diffraction XtaLAB Synergy,

Single source at offset/far, HyPix

diffractometer

Radiation source: micro-focus sealed X-ray

tube, PhotonJet (Mo) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: gaussian

CrysAlisPro (Rigaku OD, 2020)

$T_{\min} = 0.732$, $T_{\max} = 1.000$

22131 measured reflections

3686 independent reflections

3251 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.055$

$\theta_{\max} = 38.2^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -10 \rightarrow 10$

$k = -15 \rightarrow 15$

$l = -20 \rightarrow 21$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.029$ $wR(F^2) = 0.067$ $S = 1.07$

3686 reflections

110 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0285P)^2 + 0.1262P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 2.05 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.85 \text{ e } \text{\AA}^{-3}$ *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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.500000	1.000000	0.500000	0.00931 (4)
Cu1	0.250000	0.78803 (3)	0.750000	0.00868 (5)
F1	0.42425 (17)	0.82052 (11)	0.57872 (8)	0.01353 (18)
F2	0.78470 (17)	0.92222 (12)	0.46961 (9)	0.0184 (2)
F3	0.39654 (19)	0.91649 (12)	0.36083 (8)	0.0183 (2)
O1	0.4565 (2)	0.93265 (14)	0.80535 (10)	0.0147 (2)
N1	0.0722 (2)	0.62522 (16)	0.69309 (12)	0.0136 (3)
C5	0.1508 (4)	0.49153 (18)	0.71618 (16)	0.0184 (3)
C1	−0.1085 (3)	0.6393 (3)	0.63416 (16)	0.0223 (4)
H1	−0.162552	0.733418	0.618476	0.027*
C4	0.0467 (5)	0.3679 (2)	0.6778 (2)	0.0339 (6)
H4	0.103791	0.274557	0.693689	0.041*
C2	−0.2186 (4)	0.5178 (3)	0.5954 (2)	0.0357 (6)
H2	−0.347822	0.529058	0.554473	0.043*
C3	−0.1386 (5)	0.3807 (3)	0.6169 (2)	0.0438 (8)
H3	−0.210607	0.296937	0.590073	0.053*
H1A	0.424 (6)	0.983 (3)	0.864 (3)	0.037 (9)*
H1B	0.518 (6)	0.985 (3)	0.763 (3)	0.040 (10)*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01216 (7)	0.00790 (7)	0.00789 (6)	−0.00206 (4)	0.00114 (5)	0.00053 (4)
Cu1	0.00956 (11)	0.00682 (11)	0.00964 (11)	0.000	−0.00066 (9)	0.000
F1	0.0188 (5)	0.0100 (4)	0.0119 (4)	−0.0018 (3)	0.0028 (4)	0.0013 (3)
F2	0.0162 (5)	0.0176 (5)	0.0215 (5)	0.0034 (4)	0.0055 (4)	0.0071 (4)
F3	0.0284 (6)	0.0160 (5)	0.0103 (4)	−0.0102 (4)	−0.0013 (4)	−0.0008 (4)
O1	0.0188 (6)	0.0145 (6)	0.0110 (5)	−0.0075 (4)	0.0021 (4)	−0.0025 (4)
N1	0.0151 (6)	0.0130 (6)	0.0128 (6)	−0.0055 (5)	0.0019 (5)	−0.0024 (5)
C5	0.0299 (10)	0.0091 (7)	0.0166 (8)	−0.0056 (6)	0.0097 (7)	−0.0022 (5)

C1	0.0154 (8)	0.0346 (11)	0.0169 (8)	−0.0093 (7)	−0.0004 (6)	−0.0036 (7)
C4	0.0571 (16)	0.0153 (9)	0.0297 (11)	−0.0190 (9)	0.0126 (11)	−0.0078 (8)
C2	0.0306 (12)	0.0541 (16)	0.0223 (10)	−0.0294 (11)	0.0024 (9)	−0.0094 (10)
C3	0.0595 (18)	0.0433 (15)	0.0288 (11)	−0.0414 (14)	0.0116 (12)	−0.0150 (11)

Geometric parameters (Å, °)

Sn1—F1	1.9723 (10)	O1—H1B	0.81 (3)
Sn1—F1 ⁱ	1.9723 (10)	N1—C5	1.355 (2)
Sn1—F2	1.9603 (11)	N1—C1	1.337 (2)
Sn1—F2 ⁱ	1.9603 (11)	C5—C5 ⁱⁱ	1.481 (5)
Sn1—F3 ⁱ	1.9621 (10)	C5—C4	1.390 (3)
Sn1—F3	1.9621 (10)	C1—H1	0.9500
Cu1—F1	2.3830 (10)	C1—C2	1.394 (3)
Cu1—F1 ⁱⁱ	2.3830 (10)	C4—H4	0.9500
Cu1—O1 ⁱⁱ	1.9695 (12)	C4—C3	1.374 (4)
Cu1—O1	1.9695 (12)	C2—H2	0.9500
Cu1—N1 ⁱⁱ	1.9875 (14)	C2—C3	1.382 (4)
Cu1—N1	1.9875 (14)	C3—H3	0.9500
O1—H1A	0.88 (3)		
F1—Sn1—F1 ⁱ	180.0	N1 ⁱⁱ —Cu1—F1	97.98 (5)
F2—Sn1—F1 ⁱ	89.45 (4)	N1—Cu1—F1	92.92 (5)
F2 ⁱ —Sn1—F1	89.45 (4)	N1—Cu1—F1 ⁱⁱ	97.98 (5)
F2 ⁱ —Sn1—F1 ⁱ	90.55 (4)	N1 ⁱⁱ —Cu1—N1	81.95 (9)
F2—Sn1—F1	90.55 (4)	Sn1—F1—Cu1	130.20 (5)
F2 ⁱ —Sn1—F2	180.0	Cu1—O1—H1A	118 (2)
F2—Sn1—F3	89.12 (5)	Cu1—O1—H1B	120 (3)
F2 ⁱ —Sn1—F3	90.88 (5)	H1A—O1—H1B	109 (3)
F2 ⁱ —Sn1—F3 ⁱ	89.12 (5)	C5—N1—Cu1	114.47 (13)
F2—Sn1—F3 ⁱ	90.88 (5)	C1—N1—Cu1	125.42 (14)
F3 ⁱ —Sn1—F1 ⁱ	90.64 (4)	C1—N1—C5	120.09 (17)
F3 ⁱ —Sn1—F1	89.36 (4)	N1—C5—C5 ⁱⁱ	114.51 (11)
F3—Sn1—F1 ⁱ	89.36 (4)	N1—C5—C4	120.6 (2)
F3—Sn1—F1	90.64 (4)	C4—C5—C5 ⁱⁱ	124.91 (16)
F3 ⁱ —Sn1—F3	180.0	N1—C1—H1	119.5
F1—Cu1—F1 ⁱⁱ	165.56 (5)	N1—C1—C2	121.0 (2)
O1 ⁱⁱ —Cu1—F1 ⁱⁱ	84.73 (5)	C2—C1—H1	119.5
O1—Cu1—F1	84.73 (5)	C5—C4—H4	120.0
O1 ⁱⁱ —Cu1—F1	85.51 (5)	C3—C4—C5	119.9 (2)
O1—Cu1—F1 ⁱⁱ	85.51 (5)	C3—C4—H4	120.0
O1—Cu1—O1 ⁱⁱ	94.81 (8)	C1—C2—H2	120.2
O1—Cu1—N1	172.88 (6)	C3—C2—C1	119.6 (2)
O1 ⁱⁱ —Cu1—N1 ⁱⁱ	172.88 (6)	C3—C2—H2	120.2
O1—Cu1—N1 ⁱⁱ	91.70 (6)	C4—C3—C2	118.8 (2)

O1 ⁱⁱ —Cu1—N1	91.70 (6)	C4—C3—H3	120.6
N1 ⁱⁱ —Cu1—F1 ⁱⁱ	92.92 (5)	C2—C3—H3	120.6

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

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>
O1—H1 <i>A</i> $\cdots$ F2 ⁱⁱⁱ	0.88 (3)	1.79 (3)	2.6444 (17)	165 (3)
O1—H1 <i>B</i> $\cdots$ F3 ⁱ	0.81 (3)	1.84 (4)	2.6293 (17)	164 (4)

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