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# Crystal structures of three copper(II)–2,2′-bipyridine (bpy) compounds, $[Cu(bpy)_2(H_2O)][SiF_6]\cdot 4H_2O$, $[Cu(bpy)_2(TaF_6)_2]$ and $[Cu(bpy)_3][TaF_6]_2$ and a related coordination polymer, $[Cu(bpy)(H_2O)_2SnF_6]_n$

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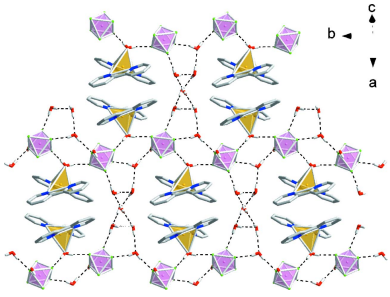
We report the hydrothermal syntheses and crystal structures of aquabis(2,2′-bipyridine-$\kappa^2N,N'$)copper(II) hexafluoridosilicate tetrahydrate, $[Cu(bpy)_2(H_2O)][SiF_6]\cdot 4H_2O$ (bpy is 2,2′-bipyridine, $C_{10}H_8N_2$), (I), bis(2,2′-bipyridine-3$\kappa^2N,N'$)-di-$\mu$-fluorido-1:3$\kappa^2F$:$F$;2:3$\kappa^2F$:$F$-decafluorido-1$\kappa^5F$,2$\kappa^5F$-ditantalum(V)copper(II), $[Cu(bpy)_2(TaF_6)_2]$, (II), tris(2,2′-bipyridine-$\kappa^2N,N'$)copper(II) bis[hexafluoridotantalate(V)], $[Cu(bpy)_3][TaF_6]_2$, (III), and *catena*-poly[[diaqua(2,2′-bipyridine-$\kappa^2N,N'$)copper(II)]-$\mu$-fluorido-tetrafluoridotin-$\mu$-fluorido], $[Cu(bpy)(H_2O)_2SnF_6]_n$, (IV). Compounds (I), (II) and (III) contain locally chiral copper coordination complexes with $C_2$, $D_2$, and $D_3$ 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 $[Cu(bpy)_2(H_2O)]^{2+}$ can crystallize in polar structures in the presence of early transition metal fluorides $MF_6^{2-}$, ($M$ = Ti, Zr, Hf) (Gautier *et al.*, 2012; Nisbet *et al.*, 2020).

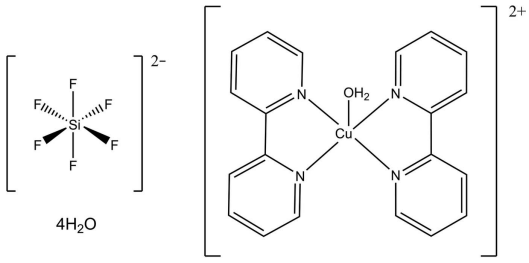
Here, we investigate the influence of the anion on the speciation of the copper(II) complex and the arrangement of the ions in the crystal structure in a series of compounds based on copper(II)–2,2′-bipyridine cations and $SiF_6^{2-}$, $SnF_6^{2-}$ and $TaF_6^{-}$ anions. Among these hydrothermally prepared structures we observe three distinct locally chiral copper-bipyridine complexes: $C_2$-symmetric cations in $[Cu(bpy)_2(H_2O)][SiF_6]\cdot 4H_2O$, (I), $D_2$-symmetric $Cu(bpy)_2(TaF_6)_2$ molecules, (II) and $D_3$-symmetric cations in $[Cu(bpy)_3][TaF_6]_2$, (III). We also report the structure of a coordination polymer based on $Cu(bpy)(H_2O)_2^{2+}$ cations and $SnF_6^{2-}$ anions, (IV), that forms under similar conditions.



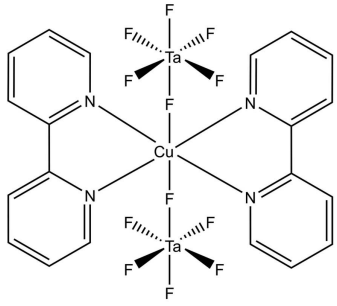

## 2. Structural commentary

Compound (I) has the formula $[Cu(bpy)_2(H_2O)][SiF_6]\cdot 4H_2O$ and crystallizes in space group $C2/c$. The structure features isolated $C_2$-symmetric Δ- and Λ-$[Cu(bpy)_2(H_2O)]^{2+}$ cations

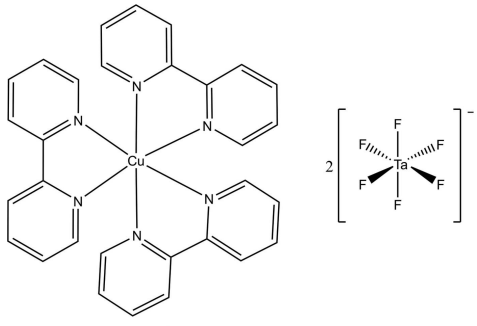
and octahedral $SiF_6^{2-}$ anions (Fig. 1). The five-coordinate $Cu^{2+}$ ion has a slightly distorted trigonal–bipyramidal coordination environment ($\tau$ = 0.77), as described by the parameter $\tau = (\beta - \alpha)/60$, where $\beta$ and $\alpha$ are the two largest angles of the complex ($\tau$ = 1 corresponds to an ideal trigonal bipyramid and $\tau$ = 0 corresponds to an ideal square pyramid) (Melnic *et al.*, 2014). The average Cu—N bond length and the Cu—$OH_2$ bond distance in (I) are in agreement with the reported distances in other known $[Cu(bpy)_2(H_2O)]^{2+}$ complexes (Gautier *et al.*, 2012; Nisbet *et al.*, 2020; Shi *et al.*, 2010; Yu *et al.*, 2007).



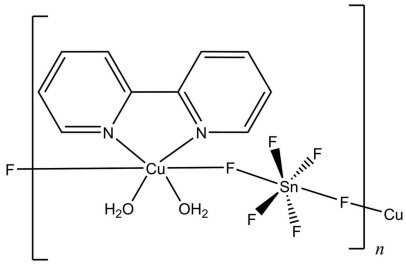

Compound (I)




Compound (II)




Compound (III)




Compound (IV)

Compound (II) has the formula $Cu(bpy)_2(TaF_6)_2$ and crystallizes in space group $P\overline{1}$. The structure is comprised of molecular Δ- and Λ- $Cu(bpy)_2(TaF_6)_2$ complexes with local $D_2$ symmetry. Each $Cu^{II}$ center is equatorially coordinated by two bpy ligands and axially coordinated by two $TaF_6^-$ groups. Two independent $Cu(bpy)_2(TaF_6)_2$ units with the same handedness are present within the arbitrarily chosen asymmetric unit (Fig. 2). These complexes differ in their Cu—F bond lengths and F—Cu—F angles: Cu1—F1 = 2.537 (3), Cu1—F7 = 2.987 (3) Å, F1—Cu1—F7 = 161.46 (9)°; Cu2—F13 =

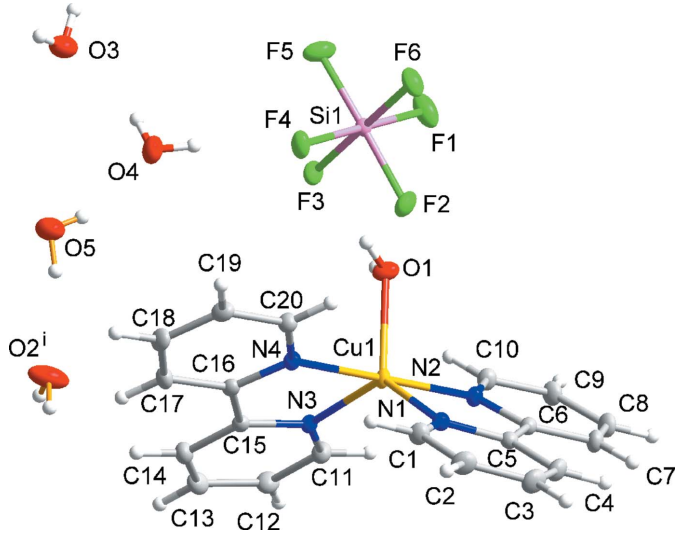



**Figure 1**
The molecular structure of (I). Ellipsoids of non-H atoms are drawn at 50% probability. H atoms are drawn with an atomic radius of 0.135 Å. [Symmetry code: (i) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$.]

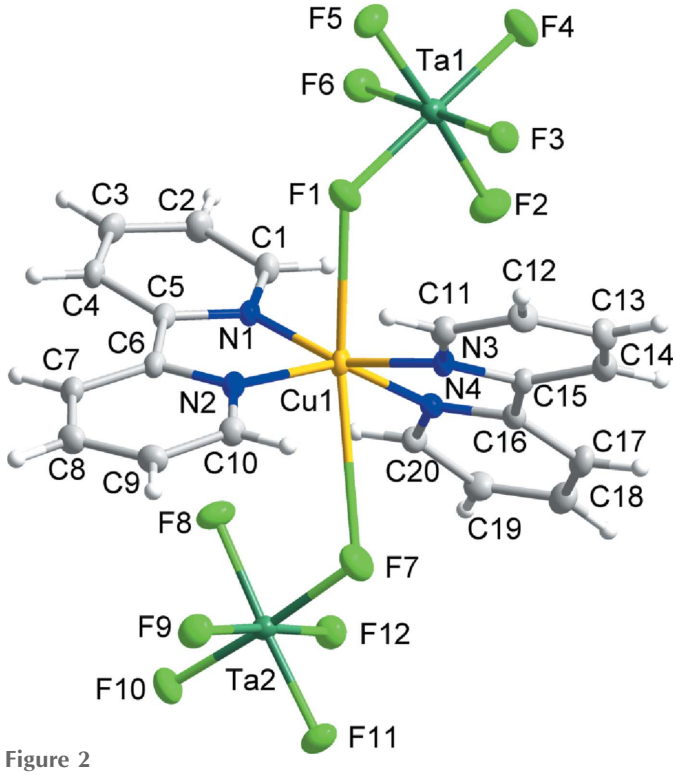



**Figure 2**
The molecular structure of one of the two independent molecules in (II). Ellipsoids of non-H atoms are drawn at 50% probability. H atoms are drawn with an atomic radius of 0.135 Å.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···F3 | 0.76 (3) | 1.91 (3) | 2.6616 (14) | 177 (3) |
| O1—H1$B$···F6$^{i}$ | 0.78 (2) | 1.93 (2) | 2.7053 (14) | 170 (2) |
| O2—H2$A$···F1 | 0.75 (2) | 1.94 (2) | 2.6677 (17) | 164 (2) |
| O2—H2$B$···F4$^{i}$ | 0.79 (3) | 2.00 (3) | 2.7807 (17) | 167 (2) |
| O3—H3$A$···F5$^{ii}$ | 0.77 (3) | 1.99 (3) | 2.7607 (18) | 177 (3) |
| O3—H3$B$···O5$^{iii}$ | 0.73 (3) | 2.06 (3) | 2.779 (2) | 171 (3) |
| O4—H4$A$···O3 | 0.72 (2) | 2.05 (2) | 2.749 (2) | 162 (2) |
| O4—H4$B$···F4 | 0.77 (3) | 1.98 (3) | 2.7462 (16) | 170 (2) |
| O5—H5$A$···O4 | 0.69 (2) | 2.13 (2) | 2.779 (2) | 158 (2) |
| O5—H5$B$···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) Å, F13—Cu2—F19 = 168.21 (10)°. 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: 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).

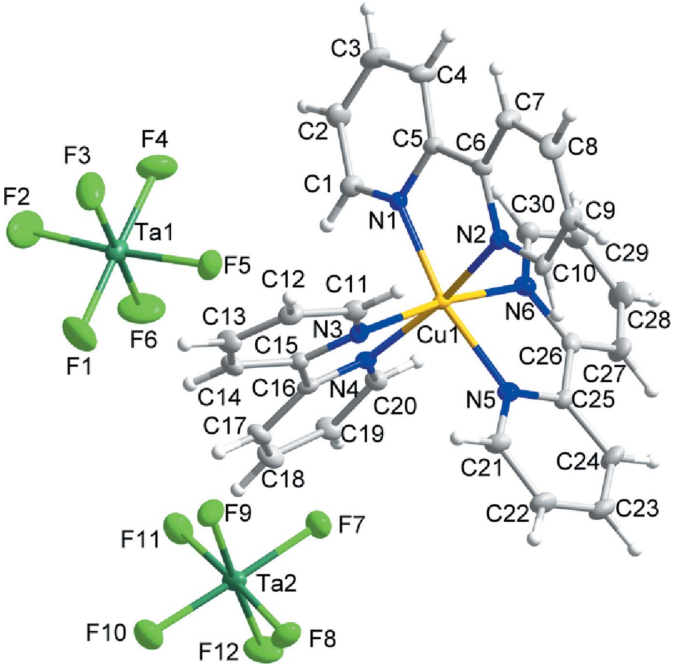



**Figure 3**
The molecular structure of (III). Ellipsoids of non-H atoms are drawn at 50% probability. H atoms are drawn with an atomic radius of 0.135 Å.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···F2$^{i}$ | 0.88 (3) | 1.79 (3) | 2.6444 (17) | 165 (3) |
| O1—H1$B$···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) $-x+1, -y+2, -z+1$.

Compound (IV) has the formula $Cu(bpy)(H_2O)_2SnF_6$ and crystallizes in space group $P2/n$. 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—H1$A$···F2 and O1—H1$B$···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 $Cu(4,4'\text{-bipyridine})_2SiF_6$ (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···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 $\pi$–$\pi$ stacking interactions between the N1/C1–C5 and N2/C6–C10 rings with an interplanar angle of 1.11 (11)°, centroid–centroid distance of 3.8774 (12) Å, and a slippage distance of 1.490 Å to form Δup–Λdown–Δup–Λdown and Δdown–Λup–Δdown–Λup chains (up/down

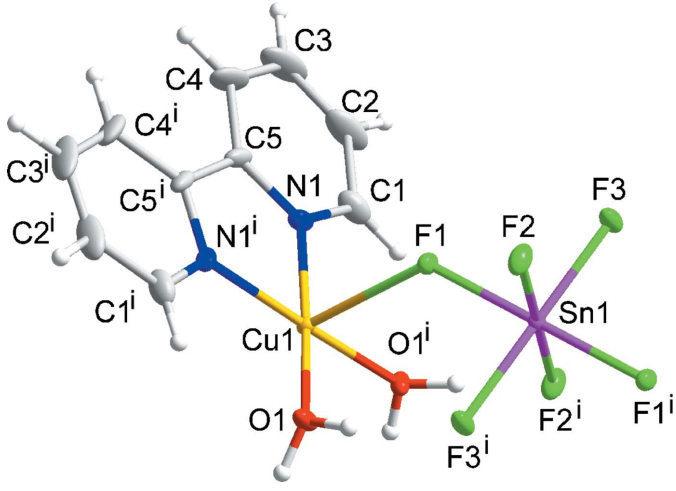



**Figure 4**
The molecular structure of (IV). Ellipsoids of non-H atoms are drawn at 50% probability. H atoms are drawn with an atomic radius of 0.135 Å. [Symmetry code: (i) $\frac{1}{2}-x, y, \frac{3}{2}-z$.]

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

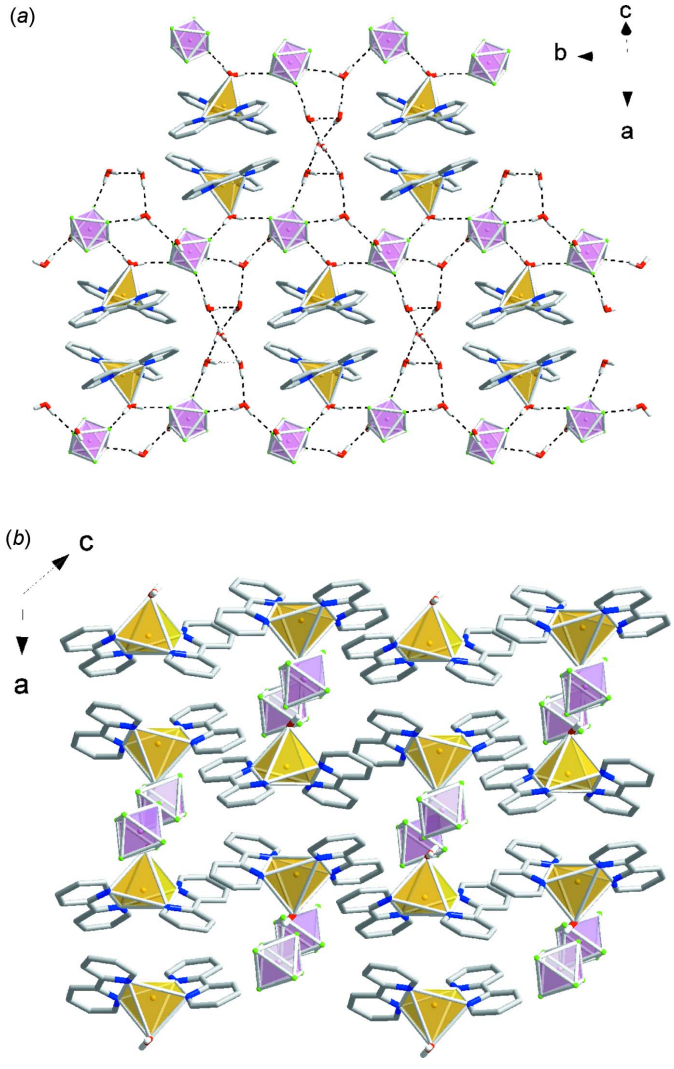



**Figure 5**
Packing diagram for (I): yellow polyhedra represent $Cu(bpy)_2(H_2O)^{2+}$ cations and pink polyhedra represent $SiF_6^{2-}$ anions.

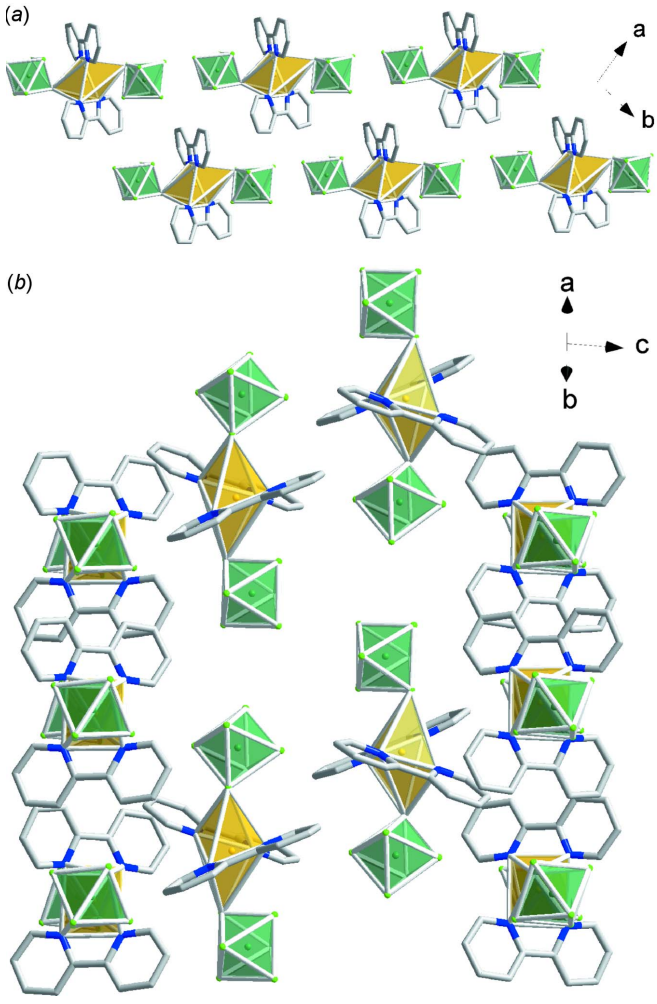



**Figure 6**
Packing diagram for (II): yellow polyhedra represent $Cu(bpy)_2^{2+}$ cations and green polyhedra represent $TaF_6^-$ anions.

The one-dimensional coordination chains in (IV) pack in a brickwork arrangement *via* parallel displaced $\pi$–$\pi$ 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) Å and a shift distance 1.676 Å, while the other stacking interaction involves nonparallel N1/C1–C5 pyridine rings with an interplanar angle of 3.54 (11)°, centroid–centroid distance of 3.5830 (14) Å and a shift distance of 1.072 Å.

## 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 $[Cu(bpy)_2(H_2O)]^{2+}$ complexes and fluorinated inorganic anions: $[Cu(bpy)_2(H_2O)][BF_4]_2$ (CSD refcode: VIKDOJ; Yu *et al.*, 2007), $[Cu(bpy)_2(H_2O)][PF_6]_2$ (CSD refcode: EQIQOL; Shi *et al.*, 2010), and $[Cu(bpy)_2(H_2O)][MF_6]$ ($M$ = Ti, Zr, Hf; CSD refcodes: GESHOD,

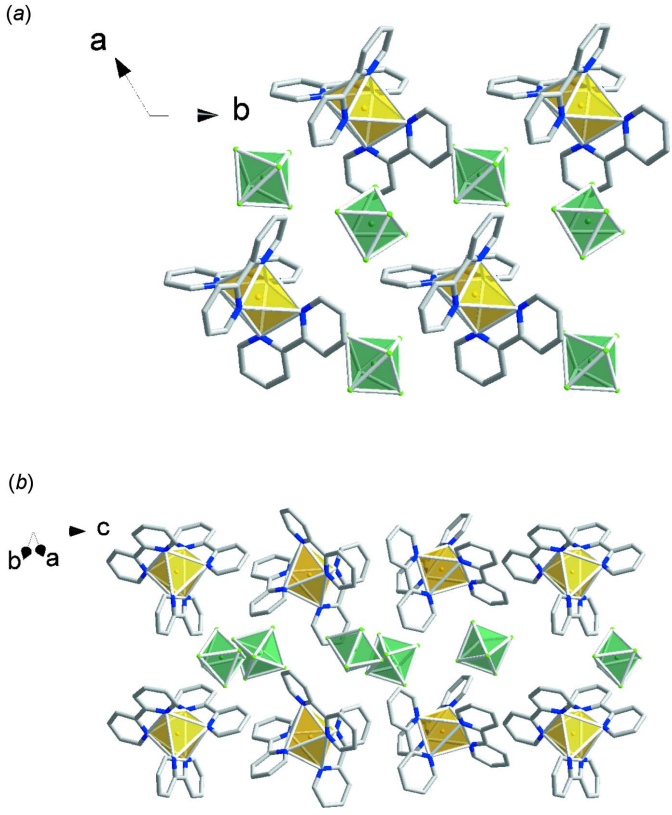



**Figure 7**
Packing diagram for (III): yellow polyhedra represent $Cu(bpy)_3^{2+}$ cations and green polyhedra represent $TaF_6^-$ anions.

YUGYEH, YUGYIL, YUGYOR; Gautier *et al.*, 2012; Nisbet *et al.*, 2020). These compounds display a variety of packing architectures, with compounds based on singly charged $PF_6^-$ 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 $[Cu(bpy)_2(H_2O)]^{2+}$ complex are both hydrogen bonded to the same pair of $[Cu(bpy)_2)(H_2O)]^{2+}$ complexes in the ETM case, whereas they are bound to two different complexes in the $SiF_6^{2-}$ case. Further, while the $[Cu(bpy)_2(H_2O)][MF_6]$ ($M$ = Ti, Zr, Hf) compounds display both face-to-face and displaced $\pi$–$\pi$ 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 $\pi$–$\pi$ stacking interactions.

Compound (III) is a new member of the family of compounds that includes $[A(bpy)_3][PF_6]$ ($A$ = Mn, Co, Ni, Cu, Zn, 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), $Zn(bpy)_3][TaF_6]_2$ (CSD refcode: HAHFII; Gautier & Poeppelmeier, 2016), and $[Zn(bpy)_3][NbF_6]_2$ (CSD refcode: HAHFUU; Gautier & Poeppelmeier, 2016). These compounds include either Δ- or Λ-$Cu(bpy)_3^{2+}$ cations arranged along $3_1$ or $3_2$ screw axes depending on the handedness of the $Cu(bpy)_3^{2+}$ complexes.

Compound (IV) is isostructural to the coordination polymer $Cu(bpy)(H_2O)HfF_6$ (CSD refcode: YUGXOQ; Nisbet *et al.*, 2020). These compounds share identical connectivity with a series of coordination polymers with the

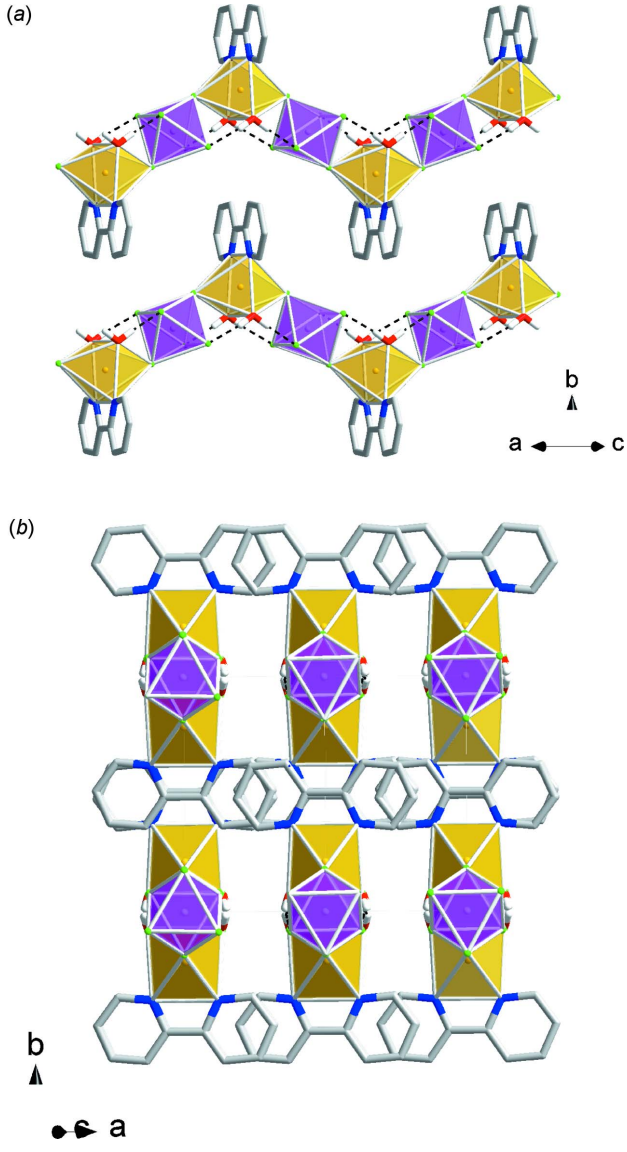



**Figure 8**
Packing diagram for (IV): Yellow polyhedra represent $Cu(bpy)(H_2O)_2^{2+}$ cations and magenta polyhedra represent $SnF_6^{2-}$ anions.

**Table 3**
Experimental details.

| | (I) | (II) | (III) | (IV) |
|---|---|---|---|---|
| Crystal data | | | | |
| Chemical formula | $[Cu(C_{10}H_8N_2)_2(H_2O)]$-$[SiF_6]\cdot 4H_2O$ | $[CuTa_2F_{12}(C_{10}H_8N_2)_2]$ | $[Cu(C_{10}H_8N_2)_3][TaF_6]_2$ | $[CuSnF_6(C_{10}H_8N_2)(H_2O)_2]$ |
| $M_r$ | 608.08 | 965.81 | 1121.99 | 488.45 |
| Crystal system, space group | Monoclinic, $C2/c$ | Triclinic, $P\overline{1}$ | Trigonal, $P3_2$ | Monoclinic, $P2/n$ |
| Temperature (K) | 100 | 100 | 100 | 100 |
| $a, b, c$ (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) |
| $\alpha, \beta, \gamma$ (°) | 90, 131.949 (1), 90 | 96.723 (1), 100.256 (1), 96.672 (1) | 90, 90, 120 | 90, 90.734 (2), 90 |
| $V$ (Å$^3$) | 4798.5 (7) | 2522.78 (5) | 2518.2 (5) | 701.70 (4) |
| $Z$ | 8 | 4 | 3 | 2 |
| Radiation type | Mo $K\alpha$ | Mo $K\alpha$ | Mo $K\alpha$ | Mo $K\alpha$ |
| $\mu$ (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 (*SADABS*; Bruker, 2016) | Gaussian *CrysAlis PRO* (Rigaku OD, 2020) | Multi-scan (*SADABS*; Bruker, 2016) | Gaussian *CrysAlis PRO* (Rigaku OD, 2020) |
| $T_{min}$, $T_{max}$ | 0.694, 0.746 | 0.035, 0.414 | 0.559, 0.746 | 0.732, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 57770, 6660, 5863 | 93570, 18263, 15170 | 148130, 12260, 12121 | 22131, 3686, 3251 |
| $R_{int}$ | 0.050 | 0.060 | 0.050 | 0.055 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.693 | 0.785 | 0.761 | 0.870 |
| Refinement | | | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 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 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.79, −0.25 | 1.67, −3.53 | 0.96, −0.85 | 2.05, −0.85 |
| Absolute structure | – | – | Flack $x$ determined using 5861 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013) | – |
| Absolute structure parameter | – | – | 0.5036 (7) | – |

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

formula $M'(bpy)(H_2O)_2MO_xF_{6-x}$ 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 $Cu(NO_3)_2\cdot H_2O$, 5 mmol of 2,2′-bipyridine, 1.5 mmol of $(NH_4)_2SiF_6$ and 1ml of deionized $H_2O$. Compound (II) was synthesized in a pouch containing 1.7 mmol of CuO, 2.5 mmol of 2,2′-bipyridine, 0.85 mmol of $Ta_2O_5$, 0.8 ml HF(aq), and 0.3 ml of deionized $H_2O$. Compound (III) was synthesized in a pouch containing 1.7 mmol of CuO, 5.1 mmol of 2,2′-bipyridine, 0.85 mmol $Ta_2O_5$, 1 ml of HF(aq) and 0.1 ml of deionized $H_2O$. Compound (IV) was synthesized in a pouch containing 1.9 mmol of $Cu(NO_3)_2\cdot H_2O$, 1.3 mmol of 2,2′-bipyridine, 1.7 mmol of $(NH_4)_2SnF_6$ and 1 ml of deionized $H_2O$.

## 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 $U_{iso}(H) = 1.2U_{eq}(C)$.

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, $[Cu(bpy)_2(H_2O)][SiF_6]\cdot 4H_2O$, $[Cu(bpy)_2(TaF_6)_2]$ and $[Cu(bpy)_3][TaF_6]_2$ and a related coordination polymer, $[Cu(bpy)(H_2O)_2SnF_6]_n$

**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-$\kappa^2N,N'$)copper(II) hexafluoridosilicate tetrahydrate (I)

*Crystal data*

$[Cu(C_{10}H_8N_2)_2(H_2O)][SiF_6]\cdot 4H_2O$
$M_r$ = 608.08
Monoclinic, *C*2/*c*
*a* = 25.4971 (16) Å
*b* = 13.3573 (9) Å
*c* = 18.944 (2) Å
*β* = 131.949 (1)°
*V* = 4798.5 (7) Å$^3$
*Z* = 8
*F*(000) = 2488
$D_x$ = 1.683 Mg m$^{-3}$
Mo *Kα* 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
$\theta_{max}$ = 29.5°, $\theta_{min}$ = 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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.79$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ e Å$^{-3}$

*Special details*

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.38373 (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, º)*

| | | | |
|---|---|---|---|
| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···F3 | 0.76 (3) | 1.91 (3) | 2.6616 (14) | 177 (3) |
| O1—H1*B*···F6$^{i}$ | 0.78 (2) | 1.93 (2) | 2.7053 (14) | 170 (2) |
| O2—H2*A*···F1 | 0.75 (2) | 1.94 (2) | 2.6677 (17) | 164 (2) |
| O2—H2*B*···F4$^{i}$ | 0.79 (3) | 2.00 (3) | 2.7807 (17) | 167 (2) |
| O3—H3*A*···F5$^{ii}$ | 0.77 (3) | 1.99 (3) | 2.7607 (18) | 177 (3) |
| O3—H3*B*···O5$^{iii}$ | 0.73 (3) | 2.06 (3) | 2.779 (2) | 171 (3) |
| O4—H4*A*···O3 | 0.72 (2) | 2.05 (2) | 2.749 (2) | 162 (2) |
| O4—H4*B*···F4 | 0.77 (3) | 1.98 (3) | 2.7462 (16) | 170 (2) |
| O5—H5*A*···O4 | 0.69 (2) | 2.13 (2) | 2.779 (2) | 158 (2) |
| O5—H5*B*···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$\kappa^2$*N*,*N*′)-di-$\mu$-fluorido-1:3$\kappa^2$*F*:*F*;2:3$\kappa^2$*F*:*F*-decafluorido-1$\kappa^5$*F*,2$\kappa^5$*F*-copper(II)ditantalum(V) (II)**

*Crystal data*

$[CuTa_2F_{12}(C_{10}H_8N_2)_2]$
$M_r$ = 965.81
Triclinic, $P\overline{1}$
*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) Å$^3$

*Z* = 4
*F*(000) = 1788
$D_x$ = 2.543 Mg m$^{-3}$
Mo *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 × 0.32 × 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$^{-1}$
$\omega$ 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 $I > 2\sigma(I)$
$R_{int}$ = 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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.67$ e Å$^{-3}$
$\Delta\rho_{min} = -3.53$ e Å$^{-3}$
Extinction correction: SHELXL-2018/3 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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) |

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|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |

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|---|---|---|---|
| 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 |

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|---|---|---|---|
| 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) |

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| 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) |

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|---|---|---|---|
| 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-$\kappa^2N,N'$)copper(II) bis[hexafluoridotantalate(V)] (III)**

*Crystal data*

$[Cu(C_{10}H_8N_2)_3][TaF_6]_2$
$M_r$ = 1121.99
Trigonal, $P3_2$
$a$ = 10.5172 (10) Å
$c$ = 26.288 (2) Å
$V$ = 2518.2 (5) Å$^3$
$Z$ = 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 × 0.16 × 0.12 mm

*Data collection*

Bruker Kappa APEX CCD area detector diffractometer
Radiation source: sealed tube
Triumph monochromator
Detector resolution: 8 pixels mm$^{-1}$
$\omega$ and $\varphi$ 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 $I > 2\sigma(I)$
$R_{int}$ = 0.050
$\theta_{max}$ = 32.7°, $\theta_{min}$ = 1.6°
$h$ = −15→15
$k$ = −15→15
$l$ = −38→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), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00031 (3)
Absolute structure: Flack $x$ determined using 5861 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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-$\kappa^2N,N'$)copper(II)]-$\mu$-fluorido-tetrafluoridotin-$\mu$-fluorido] (IV)**

*Crystal data*

| | |
|---|---|
| $[CuSnF_6(C_{10}H_8N_2)(H_2O)_2]$ | $F(000) = 470$ |
| $M_r = 488.45$ | $D_x = 2.312$ Mg m$^{-3}$ |
| Monoclinic, $P2/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 6.2590$ (2) Å | Cell parameters from 9773 reflections |
| $b = 9.2167$ (3) Å | $\theta = 2.2$–$37.7°$ |
| $c = 12.1648$ (3) Å | $\mu = 3.37$ mm$^{-1}$ |
| $\beta = 90.734$ (2)° | $T = 100$ K |
| $V = 701.70$ (4) Å$^3$ | Block, blue |
| $Z = 2$ | 0.20 × 0.13 × 0.12 mm |

*Data collection*

| | |
|---|---|
| Rigaku Oxford Diffraction XtaLAB Synergy, Single source at offset/far, HyPix diffractometer | $T_{min} = 0.732$, $T_{max} = 1.000$ |
| Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source | 22131 measured reflections |
| Mirror monochromator | 3686 independent reflections |
| Detector resolution: 10.0000 pixels mm$^{-1}$ | 3251 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int} = 0.055$ |
| Absorption correction: gaussian CrysalisPro (Rigaku OD, 2020) | $\theta_{max} = 38.2°$, $\theta_{min} = 2.2°$ |
| | $h = -10 \rightarrow 10$ |
| | $k = -15 \rightarrow 15$ |
| | $l = -20 \rightarrow 21$ |

*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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.05$ e Å$^{-3}$
$\Delta\rho_{min} = -0.85$ e Å$^{-3}$

*Special details*

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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 (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···F2$^{iii}$ | 0.88 (3) | 1.79 (3) | 2.6444 (17) | 165 (3) |
| O1—H1*B*···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.