

[SnF(bipy)(H₂O)]₂[SnF₆], a mixed-valent inorganic tin(II)–tin(IV) compound

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Received 8 July 2024
Accepted 25 July 2024

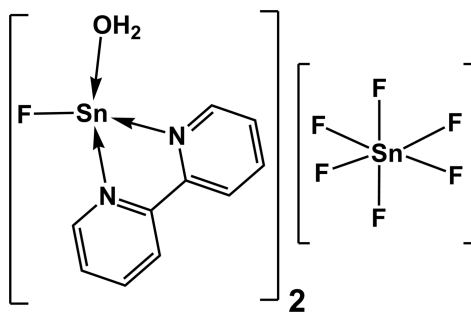
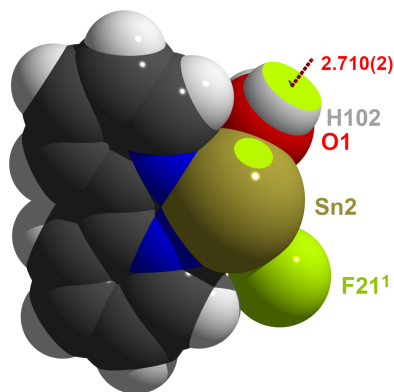
Edited by S.-L. Zheng, Harvard University, USA

Keywords: mixed-valent; hyper-valency; hydrogen bonding; dimerization; 3c–4e bonds; crystal structure.**CCDC reference:** 2373684**Supporting information:** this article has supporting information at journals.iucr.org/e

In the title compound, bis[aqua(2,2′-bipyridine)fluoridotin(II)] hexafluorido-tin(IV), [SnF(C₁₀H₈N₂)(H₂O)]₂[SnF₆], an ionic mixed-valent tin(II)–tin(IV) compound, the bivalent tin atom is the center atom of the cation and the tetravalent tin atom is the center atom of the anion. With respect to the first coordination sphere, the cation is monomeric, with the tin(II) atom having a fourfold seesaw coordination with a fluorine atom in an equatorial position, a water molecule in an axial position and the two nitrogen atoms of the chelating 2,2′-bipyridine ligand in the remaining axial and equatorial positions. The bond lengths and angles of this hypervalent first coordination sphere are described by 2c–2e and 3c–4e bonds, respectively, all of which are based on the orthogonal 5*p* orbitals of the tin atom. In the second coordination sphere, which is based on an additional, very long tin–fluorine bond that leads to dimerization of the cation, the tin atom is trapezoidal–pyramidally coordinated. The tetravalent tin atom of the centrosymmetric anion has an octahedral coordination. The differences in its tin–fluorine bond lengths are attributed to hydrogen bonding, as the two of the four fluorine atoms are each involved in two hydrogen bonds, linking anions and cations together to form strands.

1. Chemical context

Mixed-valent tin(II)–tin(IV) compounds are most often discovered by chance as a by-product of reactions in which tin(II) compounds are used as starting compounds. Two processes are discussed as potential sources of tetravalent tin (Gurnani *et al.*, 2013): the oxidation of divalent tin by atmospheric oxygen and the disproportionation of tin(II) into elemental tin and tin(IV). However, there is no evidence that the reaction proceeds in favor of either process, as the amount of the mixed-valent compound is usually limited to a few crystals. For these reasons, elemental tin is often added to the reaction mixture or an inert gas atmosphere is used.



In the case of the title compound, [SnF(H₂O)(bipy)]₂[SnF₆], in a micro-scale experiment in air (and in the absence of elemental tin), we reacted tin difluoride (SnF₂) with 2,2′-bipyridine (bipy) using *N,N*-dimethylformamide, DMF, as partial solvent and reaction mediator.

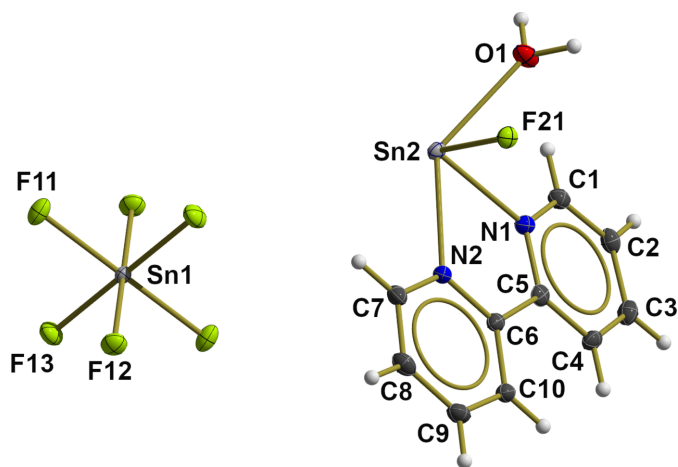


Figure 1
Ball-and-stick model of the ions found in the crystal of the title compound, showing the atom numbering of the asymmetric unit. With the exception of the H atoms, which are shown as spheres of arbitrary radius, all other atoms are drawn with displacement ellipsoids at the 50% probability level.

2. Structural commentary

The title compound crystallizes in the triclinic space group $P\bar{1}$ with half a formula unit in the asymmetric unit resulting in a centrosymmetric $[\text{Sn}^{\text{IV}}\text{F}_6]^{2-}$ anion and a $[\text{Sn}^{\text{II}}\text{F}(\text{H}_2\text{O})(\text{bipy})]^+$ cation in a general position (Fig. 1).

In the cation, the first coordination sphere of the bivalent tin atom (Fig. 2) consists of one fluorine atom, the oxygen atom of the water molecule and both nitrogen atoms of the 2,2'-bipyridine ligand. In this seesaw coordination, the fluorine atom [$d(\text{Sn}-\text{F}) = 2.022(1) \text{ \AA}$] adopts an equatorial (*eq*) position and the water molecule [$d(\text{Sn}-\text{O}) = 2.408(2) \text{ \AA}$] an axial (*ax*) one, while the nitrogen atoms of the chelating 2,2'-

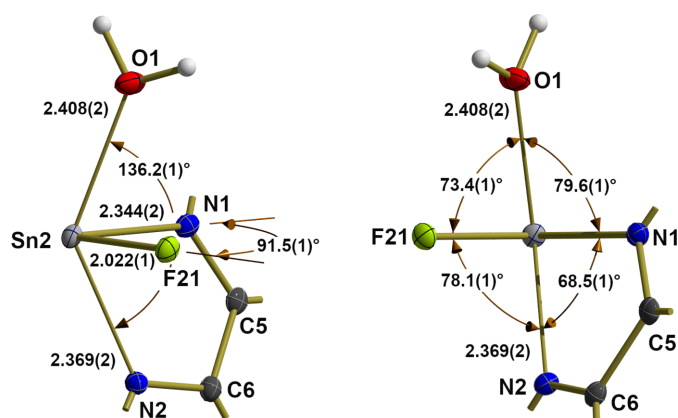


Figure 2
Ball-and-stick model (left: side view; right: front view) of the first, seesaw coordination sphere of the bivalent tin atom Sn2 of the cation, highlighting selected bond lengths (\AA) and angles ($^\circ$). With the exception of the H atoms, which are shown as spheres of arbitrary radius, all other atoms are drawn with displacement ellipsoids at the 50% probability level. For clarity, only the carbon atoms between the two nitrogen atoms of the bipyridine ligand are shown, the position of all other carbon atoms are indicated as shortened sticks. Axial bonds are drawn as sticks of reduced thickness in order to underline the presence of a $3c-4e$ bond.

bipyridine ligand occupy the two other axial and equatorial positions. According with this arrangement, both tin–nitrogen distances differ [$0.025(1) \text{ \AA}$] with the shorter one to N_{eq} [$2.344(2) \text{ \AA}$] and the longer one to N_{ax} [$2.369(2) \text{ \AA}$].

Within the equatorial plane, the $\text{N}_{eq}-\text{Sn}-\text{F}$ bond angle is $91.5(1)^\circ$, whereas the axis is clearly bent [$136.2(1)^\circ$]. Among the axial-to-equatorial bond angles, the bond angle between the nitrogen atoms is very acute [$68.5(1)^\circ$] due to the steric restrictions of the ligand. Conspicuously, the bond angle *trans* to this chelating bond angle is also quite acute [$73.4(1)^\circ$] while the other two are much more obtuse [$78.1(1)^\circ$, $79.6(1)^\circ$].

In the VB concept with its localized $2c-2e$ bonds, the bond ratios within the cation are difficult to describe because the tin atom with its non-bonding $5s$ electron pair and the eight electrons of the four donor atoms (F^- , O , N , N) exceeds the electron octet of a main group element. In contrast, the MO theory according to Pimentel and Rundle (Pimentel, 1951; Rundle, 1949) provides a simple and logical explanation for this hyper-valence in the form of a $3c-4e$ bond with the exclusive participation of p orbitals on all three atoms. In a seesaw-shaped coordination geometry, this $3c-4e$ bond is usually found in the axially arranged atoms, while the atoms in the equatorial plane are bonded *via* $2c-2e$ bonds through the other p orbitals of the tin atom. This bonding concept not only explains the different tin–nitrogen bond lengths, but also the bond angles around or smaller than 90° as a result of the orthogonality of the tin p -orbitals. It also explains the remarkable long [$2.408(2) \text{ \AA}$] tin–oxygen distance to the water molecule, for which bond lengths between $2.207(2) \text{ \AA}$ and $2.226(2) \text{ \AA}$ [mean value: $2.226(17) \text{ \AA}$] are observed (Kleeberg *et al.*, 2022) in electron-precise tin(II) compounds of the type $[\text{Sn}(\text{OH}_2)_3]^{2+}$ with the tin atom at the apex of a

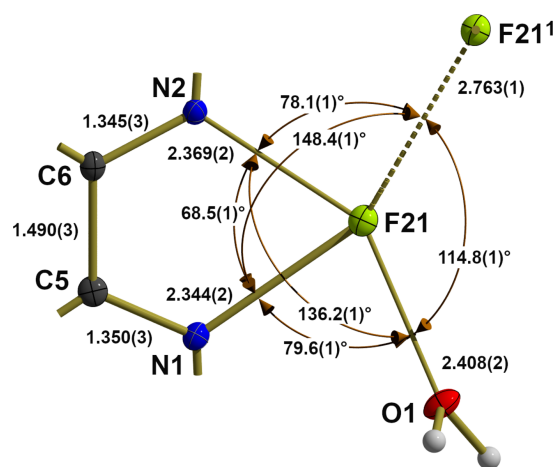


Figure 3
Ball-and-stick model of the second, trapezoid-pyramidal coordination sphere of Sn2, highlighting selected bond lengths (\AA) and angles ($^\circ$), viewed down the fluorine–tin bond. With the exception of the H atoms, which are shown as spheres of arbitrary radius, all other atoms are drawn with displacement ellipsoids at the 50% probability level. For clarity, only the carbon atoms between the two nitrogen atoms of the bipyridine ligand are shown, the position of all other carbon atoms are indicated as shortened sticks. Axial bonds are drawn as sticks of reduced thickness in order to underline the presence of a $3c-4e$ bond, as is the additional asymmetric $3c-4e$ bond shown with a dashed line. Symmetry code: (i) $-x, -y, 1-z$.

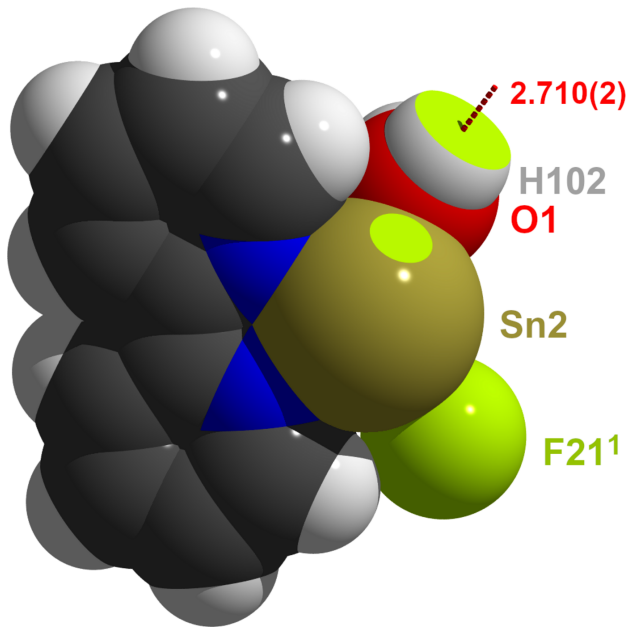


Figure 4
Space-filling model of the $[\text{SnF}(\text{bipy})(\text{H}_2\text{O})]^+$ cation looking down the *apical* tin–fluorine bond and visualizing the hemi-directed coordination of the bivalent tin atom Sn2. Atoms whose spheres are penetrated by other atoms are visualized as truncated two-colored spheres, the hydrogen bond is indicated by a dashed red line. Atom colors and van der Waals radii (Å) are as follows: F = green/1.47, H = white/1.10, C = gray/1.70, O = red/1.52, N = blue/1.55 and Sn = brass/2.17. Symmetry code: (i) $-x, -y, 1 - z$.

trigonal pyramid and the three oxygen atoms of the water molecules at its base.

If only the first coordination sphere is taken as a basis, the cation is monomeric. However, there is a second monomer in its immediate vicinity, whereby both are in contact with each other *via* a long tin–fluorine bridge [$d(\text{Sn}–\text{F}) = 2.763(1) \text{ \AA}$] resulting from a center of symmetry (Fig. 3). This additional,

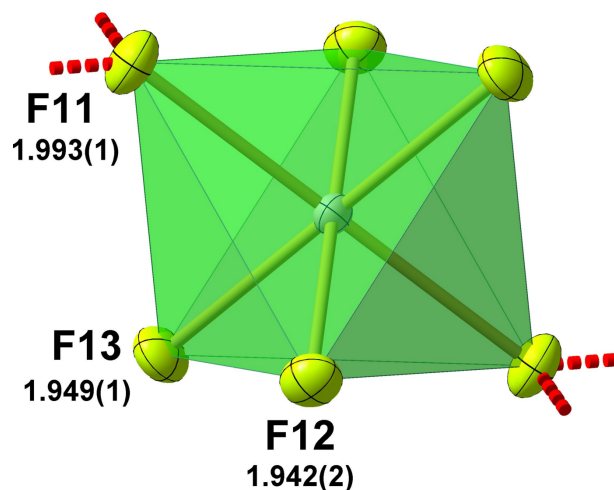


Figure 5
Polyhedron and ball-and-stick model of the octahedral, centrosymmetric $[\text{SnF}_6]^{2-}$ anion with bond lengths (Å) and hydrogen bonds indicated by dashed red lines. All atoms are drawn with displacement ellipsoids at the 50% probability level.

weak bond is in the *trans* position [$(\text{N}–\text{Sn}–\text{F}) = 148.4(1)^\circ$] to the original, *equatorial* tin–nitrogen bond and extends the seesaw-shaped, fourfold coordination of the two tin atoms to fivefold, pyramidal coordinations, in which the tin atoms are each below [$\Delta_{\text{least-squares}} = -0.6035(1) \text{ \AA}$] the trapezoidal, strongly uneven [$\pm\Delta_{\text{max, least-squares}} = -0.147(1)/0.138(1) \text{ \AA}$] base while the shortest bonds [$d(\text{Sn}–\text{F}) = 2.022(1) \text{ \AA}$] point in the direction of the *apical* fluorine atoms. This dimerization leads to a bridging angle of $111.8(1)^\circ$ at the fluorine atoms and a four-membered, centrosymmetric and therefore exactly planar tin–fluorine ring. Its rhomboidal shape is characterized by acute [$68.2(1)^\circ$] angles at the tin atoms and obtuse [$111.8(1)^\circ$] ones at the fluorine atoms. Extending the Pimentel–Rundle concept, Musher (1969) suggests that such additional, very weak bonds result from a *p* orbital of the central atom, that is involved in a classical $2c-2e$ bond on the one hand and a $3c-4e$ bond on the other. As result, in such ‘asymmetric’ $3c-4e$ bonds, one ligand is much more strongly bound to the central atom than the *trans*-ligand. Despite this additional bond, the coordination sphere of the tin atom (Fig. 4) remains hemi-directed (Shimoni-Livny *et al.*, 1998).

The octahedral shape of the centrosymmetric $[\text{SnF}_6]^{2-}$ anion is reflected in bond angles around 90° [$88.4(1)–91.6(1)^\circ$] and very similar tin–fluorine bond lengths. While four of the bonds (F12, F13) are almost identical in length [$1.949(1)/1.942(2) \text{ \AA}$], two bonds (F11) are somewhat longer [$1.993(1) \text{ \AA}$] because the fluorine atoms undergo hydrogen bonding with the hydrogen atoms of two different water molecules (Fig. 5).

3. Supramolecular features

Similar to the expansion of the coordination spheres of the bivalent tin atoms through further, asymmetric $3c-4e$ bonds, the hydrogen bonds between the water molecules of the cation

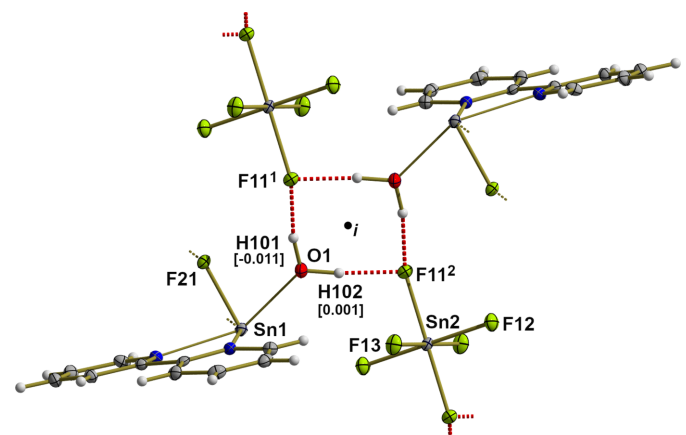


Figure 6
Ball-and-stick model showing in detail the hydrogen-bonding scheme between cation and anion (dashed red lines). With the exception of the H atoms, which are shown as spheres of arbitrary radius, all other atoms are drawn with displacement ellipsoids at the 50% probability level. The out-of-plane deflections (Å) of the hydrogen atoms are given in square brackets, *i* = center of symmetry. Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $x, y, z - 1$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H101 \cdots F11 ⁱ	0.96	1.75	2.705 (2)	170
O1–H102 \cdots F11 ⁱⁱ	0.96	1.75	2.710 (2)	174

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

and the fluorine atoms of the anion play a central role in the formation of the crystal structure. Both hydrogen atoms of the water molecule but only one fluorine atom of the anion are involved in these hydrogen bonds whereby a centrosymmetric, almost planar, eight-membered $-O-H\cdots F$ ring is formed (Fig. 6). The geometries of the two crystallographic independent hydrogen bonds are given in Table 1. The out-of-plane deflections of the H atoms are $+0.011$ Å for H101 and -0.001 Å for H102. As a result of these hydrogen bonds, the anions and cations are arranged into strands that expand in the a -axis direction (Fig. 7).

4. Database survey

The $[\text{SnF}_6]^{2-}$ anion is often a component of salts with organic and inorganic cations. While in combination with inorganic cations the tin–fluorine distances are often strongly influenced by the cation–anion interactions [*i.e.* Na_2SnF_6 : $d(\text{Sn}-\text{F}) = 1.958$ Å; Benner & Hoppe, 1990], very similar bond lengths [$d_{\text{mean}}(\text{Sn}-\text{F})$ without/with hydrogen bonds: 1.938 (2)/1.956 (2) Å, 24/16 values] to the title compound are found in combination with organic cations (Lermontov *et al.*, 2010; Bouacida *et al.*, 2005; Taha *et al.*, 1992; Cortijo *et al.*, 2017; Kokunov *et al.*, 2007; Jung *et al.*, 2023).

Isolated monomeric or dimeric cations of the type $[\text{Sn}^{\text{II}}\text{F}(\text{LB}^0)_3]^+$ or $[\text{Sn}^{\text{II}}\text{F}(\text{LB}^0)_2]^+$ with $\text{LB}^0 =$ neutral Lewis base have not yet been described in the literature, but a comparable mixed-valent tin(II)–tin(IV) compound also from

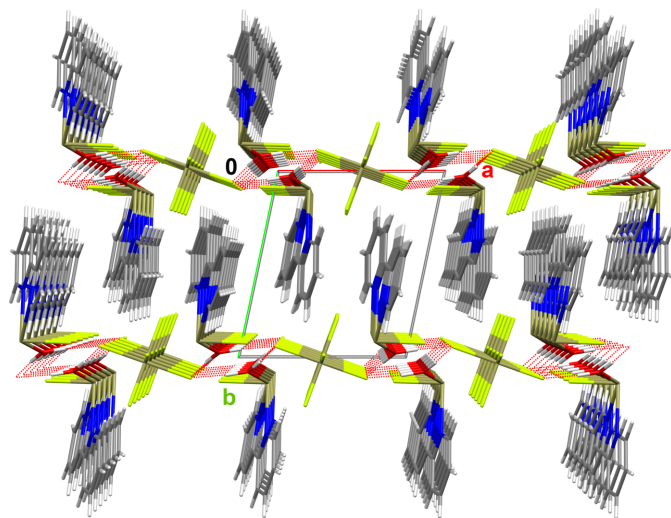


Figure 7
Stick model of the crystal packing looking down the crystallographic c axis and showing the strands resulting from the hydrogen bonds (dashed red lines) between anions and cations. Color code as in Fig. 4.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[\text{SnF}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2][\text{SnF}_6]$
M_r	856.47
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	7.4579 (4), 8.4601 (5), 9.8864 (6)
α, β, γ (°)	97.073 (2), 98.474 (2), 100.644 (2)
V (Å ³)	599.06 (6)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	3.19
Crystal size (mm)	0.17 × 0.15 × 0.05
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
$T_{\text{min}}, T_{\text{max}}$	0.434, 0.713
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28904, 2864, 2611
R_{int}	0.063
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.660
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.022, 0.053, 1.05
No. of reflections	2864
No. of parameters	172
H-atom treatment	Only H-atom displacement parameters refined
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.89, -0.69

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2006), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

SnF_2 and 2,2'-bipyridine was previously described by Gurnani *et al.* (2013): $[\text{SnF}(\text{bipy})_2][\text{SnF}_6]$. In this compound, the first coordination sphere of the bivalent tin atom exhibits a four-fold, seesaw $\{\text{SnN}_2\text{F}_2\}$ coordination with one additional, axial fluorine atom [$d(\text{Sn}-\text{F}) = 2.510$ (2) Å] instead of the axial water molecule in the title compound and similar tin–fluorine [$d(\text{Sn}-\text{F})_{\text{eq}} = 2.031$ (2) Å] and tin–nitrogen distances [$d(\text{Sn}-\text{N})_{\text{eq}} = 2.298$ (3) Å, $d(\text{Sn}-\text{N})_{\text{ax}} = 2.335$ (3) Å]. As in the title compound, dimerization proceeds *via* an asymmetrical $3c-4e$ bond [$d(\text{Sn}\cdots\text{F}_{\text{eq}}) = 2.738$ (3) Å], generating a similar, centrosymmetric four-membered Sn–F ring and trapezoid–pyramidally coordinated tin atoms. Regarding the centrosymmetric $[\text{SnF}_6]^{2-}$ anion of this compound, the Sn–F distances are 1.956 (3) and 1.944 (3) Å for the terminal fluorine atoms and 1.995 (3) Å in case of the μ_2 -fluorine atom that adopts the *axial* position in the first coordination sphere of the bivalent tin atom.

5. Synthesis and crystallization

A mixture of approximately 157 mg (1 mmol) of SnF_2 (Aldrich) and 156 mg (1 mmol) of 2,2'-bipyridine (Sigma Aldrich) was placed in a Petri dish and 5 ml of *N,N*-dimethylformamide (Sigma Aldrich) were added *via* a syringe. No elemental tin was added, nor was oxygen from the air excluded. The following processes were observed from day to day with a light microscope (Stemi 1000, Zeiss, Oberkochen, Germany). After two days small, colorless, block-like crystals

of the title compound appeared, which, after two additional days, reached a size that was sufficient for a single crystal X-ray determination.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The positions of all H atoms were clearly identified in difference-Fourier maps. Those of the organic ligand were refined with calculated positions (C–H = 0.93 Å) and a common isotropic displacement parameter. The positions of the H atoms of the water molecule were refined with a fixed O–H distance of 0.96 Å and a bond angle of 104.95° before they were fixed and allowed to ride on the parent O atom with an isotropic displacement parameter.

Acknowledgements

The Deutsche Forschungsgemeinschaft and the Government of Lower-Saxony are thanked for the funding of the diffractometer.

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supporting information

Acta Cryst. (2024). E80, 921-925 [https://doi.org/10.1107/S2056989024007400]

[SnF(bipy)(H₂O)]₂[SnF₆], a mixed-valent inorganic tin(II)–tin(IV) compound

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Computing details

Bis[aqua(2,2'-bipyridine)fluoridotin(II)] hexafluoridotin(IV)

Crystal data

[SnF(C₁₀H₈N₂)(H₂O)]₂[SnF₆]

$M_r = 856.47$

Triclinic, $P\bar{1}$

$a = 7.4579$ (4) Å

$b = 8.4601$ (5) Å

$c = 9.8864$ (6) Å

$\alpha = 97.073$ (2)°

$\beta = 98.474$ (2)°

$\gamma = 100.644$ (2)°

$V = 599.06$ (6) Å³

$Z = 1$

$F(000) = 406$

$D_x = 2.374$ Mg m⁻³

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

Cell parameters from 9888 reflections

$\theta = 2.5$ – 28.9 °

$\mu = 3.19$ mm⁻¹

$T = 100$ K

Plate, colourless

$0.17 \times 0.15 \times 0.05$ mm

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.434$, $T_{\max} = 0.713$

28904 measured reflections

2864 independent reflections

2611 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.063$

$\theta_{\max} = 28.0$ °, $\theta_{\min} = 3.0$ °

$h = -9 \rightarrow 9$

$k = -10 \rightarrow 11$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.053$

$S = 1.05$

2864 reflections

172 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Hydrogen site location: mixed

Only H-atom displacement parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.024P)^2 + 0.4078P]$

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

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

$\Delta\rho_{\max} = 0.89$ e Å⁻³

$\Delta\rho_{\min} = -0.69$ e Å⁻³

Extinction correction: *SHELXL2014/7*

(Sheldrick, 2015),

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

Extinction coefficient: 0.0061 (6)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.5000	1.0000	1.0000	0.01059 (8)
F11	0.22638 (19)	0.91895 (18)	0.96683 (15)	0.0190 (3)
F12	0.5060 (2)	0.96203 (18)	0.80238 (14)	0.0192 (3)
F13	0.4618 (2)	1.21909 (17)	0.98795 (15)	0.0198 (3)
Sn2	0.21949 (2)	0.11033 (2)	0.42958 (2)	0.01159 (8)
F21	−0.05571 (18)	0.10252 (17)	0.41199 (14)	0.0143 (3)
N1	0.2719 (3)	0.3727 (2)	0.3702 (2)	0.0124 (4)
C1	0.3234 (3)	0.3987 (3)	0.2477 (3)	0.0150 (5)
H1	0.3362	0.3083	0.1854	0.015 (2)*
C2	0.3578 (3)	0.5513 (3)	0.2103 (2)	0.0161 (6)
H2	0.3939	0.5660	0.1237	0.015 (2)*
C3	0.3388 (3)	0.6832 (3)	0.3011 (3)	0.0169 (5)
H3	0.3597	0.7895	0.2769	0.015 (2)*
C4	0.2890 (3)	0.6585 (3)	0.4277 (3)	0.0149 (5)
H4	0.2761	0.7477	0.4914	0.015 (2)*
C5	0.2581 (3)	0.5018 (3)	0.4601 (2)	0.0125 (5)
C6	0.2159 (3)	0.4654 (3)	0.5971 (2)	0.0120 (5)
N2	0.2082 (3)	0.3096 (2)	0.6171 (2)	0.0118 (4)
C7	0.1811 (3)	0.2676 (3)	0.7394 (2)	0.0152 (5)
H7	0.1791	0.1582	0.7534	0.015 (2)*
C8	0.1557 (4)	0.3780 (3)	0.8464 (3)	0.0174 (5)
H8	0.1343	0.3447	0.9319	0.015 (2)*
C9	0.1622 (3)	0.5373 (3)	0.8268 (3)	0.0167 (5)
H9	0.1450	0.6151	0.8991	0.015 (2)*
C10	0.1940 (3)	0.5838 (3)	0.7003 (2)	0.0135 (5)
H10	0.2006	0.6934	0.6852	0.015 (2)*
O1	0.0938 (2)	0.0501 (2)	0.18594 (17)	0.0187 (4)
H101	−0.0229	0.0670	0.1412	0.073 (10)*
H102	0.1481	0.0034	0.1126	0.073 (10)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.00996 (13)	0.01193 (14)	0.01123 (13)	0.00387 (9)	0.00360 (9)	0.00239 (9)
F11	0.0116 (7)	0.0237 (8)	0.0199 (8)	0.0027 (6)	0.0030 (6)	−0.0024 (6)
F12	0.0216 (8)	0.0231 (8)	0.0133 (7)	0.0042 (6)	0.0053 (6)	0.0027 (6)
F13	0.0255 (8)	0.0155 (8)	0.0224 (8)	0.0096 (6)	0.0069 (6)	0.0062 (6)
Sn2	0.01071 (11)	0.01044 (11)	0.01397 (12)	0.00390 (7)	0.00208 (7)	0.00069 (7)
F21	0.0110 (7)	0.0161 (7)	0.0165 (7)	0.0044 (5)	0.0035 (5)	0.0015 (6)

N1	0.0104 (10)	0.0133 (10)	0.0134 (10)	0.0023 (8)	0.0027 (8)	0.0004 (8)
C1	0.0130 (12)	0.0165 (13)	0.0145 (13)	0.0023 (10)	0.0017 (10)	0.0009 (10)
C2	0.0120 (13)	0.0223 (15)	0.0150 (14)	0.0043 (11)	0.0022 (11)	0.0054 (12)
C3	0.0146 (12)	0.0152 (13)	0.0214 (14)	0.0020 (10)	0.0025 (10)	0.0071 (11)
C4	0.0138 (12)	0.0124 (12)	0.0186 (13)	0.0050 (9)	0.0019 (10)	0.0003 (10)
C5	0.0066 (11)	0.0152 (12)	0.0161 (12)	0.0031 (9)	0.0020 (9)	0.0023 (10)
C6	0.0091 (11)	0.0115 (12)	0.0145 (12)	0.0020 (9)	0.0004 (9)	0.0009 (10)
N2	0.0128 (10)	0.0107 (10)	0.0111 (10)	0.0024 (8)	0.0003 (8)	0.0010 (8)
C7	0.0156 (12)	0.0148 (12)	0.0132 (12)	0.0008 (10)	-0.0010 (10)	0.0024 (10)
C8	0.0168 (13)	0.0225 (14)	0.0118 (12)	0.0012 (10)	0.0026 (10)	0.0027 (11)
C9	0.0156 (12)	0.0190 (13)	0.0141 (13)	0.0044 (10)	0.0014 (10)	-0.0027 (10)
C10	0.0136 (12)	0.0121 (12)	0.0142 (12)	0.0032 (9)	0.0009 (9)	0.0000 (10)
O1	0.0162 (9)	0.0269 (10)	0.0132 (9)	0.0068 (8)	0.0037 (7)	-0.0016 (8)

Geometric parameters (Å, °)

Sn1—F13	1.9418 (14)	C3—H3	0.9500
Sn1—F13 ⁱ	1.9418 (14)	C4—C5	1.389 (3)
Sn1—F12 ⁱ	1.9491 (14)	C4—H4	0.9500
Sn1—F12	1.9491 (14)	C5—C6	1.490 (3)
Sn1—F11	1.9931 (14)	C6—N2	1.349 (3)
Sn1—F11 ⁱ	1.9931 (14)	C6—C10	1.389 (3)
Sn2—F21	2.0221 (13)	N2—C7	1.335 (3)
Sn2—N1	2.344 (2)	C7—C8	1.381 (4)
Sn2—N2	2.369 (2)	C7—H7	0.9500
Sn2—O1	2.4076 (17)	C8—C9	1.378 (4)
N1—C5	1.350 (3)	C8—H8	0.9500
N1—C1	1.354 (3)	C9—C10	1.396 (3)
C1—C2	1.375 (3)	C9—H9	0.9500
C1—H1	0.9500	C10—H10	0.9500
C2—C3	1.386 (3)	O1—H101	0.9600
C2—H2	0.9500	O1—H102	0.9600
C3—C4	1.385 (4)		
F13—Sn1—F13 ⁱ	180.0	C4—C3—C2	119.3 (2)
F13—Sn1—F12 ⁱ	89.28 (6)	C4—C3—H3	120.3
F13 ⁱ —Sn1—F12 ⁱ	90.72 (6)	C2—C3—H3	120.3
F13—Sn1—F12	90.72 (6)	C3—C4—C5	119.1 (2)
F13 ⁱ —Sn1—F12	89.28 (6)	C3—C4—H4	120.4
F12 ⁱ —Sn1—F12	180.00 (9)	C5—C4—H4	120.4
F13—Sn1—F11	89.59 (6)	N1—C5—C4	121.6 (2)
F13 ⁱ —Sn1—F11	90.41 (6)	N1—C5—C6	115.7 (2)
F12 ⁱ —Sn1—F11	88.39 (6)	C4—C5—C6	122.7 (2)
F12—Sn1—F11	91.61 (6)	N2—C6—C10	121.7 (2)
F13—Sn1—F11 ⁱ	90.41 (6)	N2—C6—C5	115.3 (2)
F13 ⁱ —Sn1—F11 ⁱ	89.59 (6)	C10—C6—C5	122.9 (2)
F12 ⁱ —Sn1—F11 ⁱ	91.62 (6)	C7—N2—C6	119.5 (2)
F12—Sn1—F11 ⁱ	88.39 (6)	C7—N2—Sn2	120.78 (16)

F11—Sn1—F11 ⁱ	180.00 (3)	C6—N2—Sn2	119.55 (15)
F21—Sn2—N1	91.52 (6)	N2—C7—C8	122.1 (2)
F21—Sn2—N2	78.11 (6)	N2—C7—H7	118.9
N1—Sn2—N2	68.50 (7)	C8—C7—H7	118.9
F21—Sn2—O1	73.42 (6)	C9—C8—C7	118.8 (2)
N1—Sn2—O1	79.62 (6)	C9—C8—H8	120.6
N2—Sn2—O1	136.22 (6)	C7—C8—H8	120.6
C5—N1—C1	118.7 (2)	C8—C9—C10	119.7 (2)
C5—N1—Sn2	120.40 (15)	C8—C9—H9	120.2
C1—N1—Sn2	120.81 (16)	C10—C9—H9	120.2
N1—C1—C2	122.4 (2)	C6—C10—C9	118.1 (2)
N1—C1—H1	118.8	C6—C10—H10	121.0
C2—C1—H1	118.8	C9—C10—H10	121.0
C1—C2—C3	118.8 (2)	Sn2—O1—H101	127.2
C1—C2—H2	120.6	Sn2—O1—H102	127.9
C3—C2—H2	120.6	H101—O1—H102	105.0

Symmetry code: (i) $-x+1, -y+2, -z+2$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H101 \cdots F11 ⁱⁱ	0.96	1.75	2.705 (2)	170
O1—H102 \cdots F11 ⁱⁱⁱ	0.96	1.75	2.710 (2)	174

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