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Strontium hexafluoridostannate(IV) dihydrate

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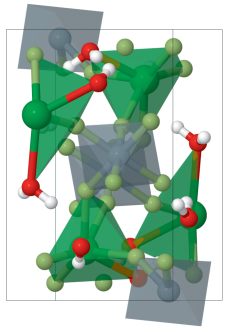
Colourless, needle-like single crystals of the title compound, $Sr[SnF_6]\cdot 2H_2O$, were grown from stoichiometric amounts of SrF_2 and SnF_4 in boiling water. The compound is isostructural with the corresponding hexafluoridoiridate(IV) and features a nearly undistorted octahedral $[SnF_6]^{2-}$ anion with C_1 point-group symmetry, as well as an Sr^{2+} ion in a distorted, square-antiprismatic coordination environment. The resulting $[SrF_5(H_2O)_3]$ coordination polyhedra share an edge *via* two water molecules to form centrosymmetric dimers. As the strength of the O—H···F and O—H···O hydrogen bonds is less pronounced, the crystal packing is dominated by μ_2-F atoms between anions and cations.

3D view



Structure description

Hexafluoridostannates(IV), $[SnF_6]^{2-}$, with monovalent and divalent metal cations have long been known (Marignac, 1859). They occur in both hydrated and anhydrous forms. Although they have frequently been studied crystallographically in the past (*e.g.* Hoppe *et al.*, 1972; Lari Lavassani *et al.*, 1974), complete, high-resolution single-crystal data sets based on diffractometer data are rare. $Fe[SnF_6]\cdot 6H_2O$ belongs to this group (Denes *et al.*, 1994), but as its atomic coordinates have not been published or deposited, it cannot be found in any of the crystallographic databases. The situation is somewhat better in the case of simple ammonium and phosphonium cations like $(Me_3NH)^+$ (dihydrate; Taha *et al.*, 1992) or $(Ph_4P)^+$ (anhydrous; Cortijo *et al.*, 2018). Today, the $[SnF_6]^{2-}$ anion is becoming increasingly important as a building block in coordination polymers (Li *et al.*, 2024; Wang *et al.*, 2024; Xiong *et al.*, 2024).

The title compound, strontium hexafluoridostannate(IV) dihydrate, is isostructural with the corresponding hexafluoridoiridate(IV) of strontium (Smolentsev *et al.*, 2007). In the $[SnF_6]^{2-}$ anion, point-group symmetry C_1, Fig. 1, the tin–fluorine distances vary between 1.9356 (14) and 1.9573 (13) Å, mean value = 1.947 (10) Å, whilst the bond angles between the *trans* oriented fluorine atoms are 176.38 (6), 176.81 (6), and 177.37 (6)°. In other cases, these bond angles are exactly 180°, as the anion exhibits higher symmetry, and the Sn—F bond lengths are somewhat shorter as reported in older,

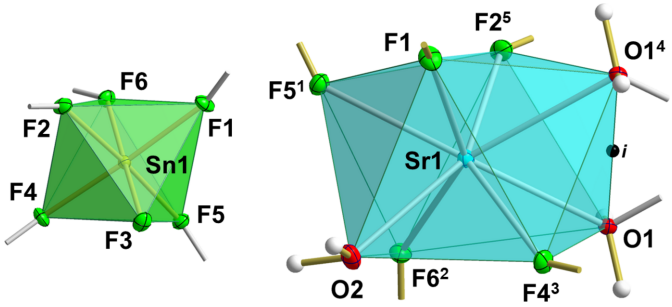


Figure 1
Coordination polyhedra around the metal atoms in $Sr[SnF_6]\cdot 2H_2O$ with atom numbering. The almost octahedral $[SnF_6]^{2-}$ anion (green, left) and the distorted square-antiprismatic $[SrF_5(H_2O)_3]$ polyhedron (blue, right) are on the same scale with all non-H atoms drawn as displacement ellipsoids at the 50% probability level. Covalent bonds are drawn in bronze, coordinative bonds are drawn in grey; the black dot labelled *i* indicates the position of the centre of symmetry generating the dimers of the strontium coordination polyhedra. [Symmetry codes: (1) $1-x,1-y,1-z$; (2) $\frac{1}{2}+x,\frac{3}{2}-y,-\frac{1}{2}+z$; (3) $\frac{3}{2}-x,\frac{1}{2}+y,\frac{3}{2}-z$; (4) $1-x,2-y,1-z$; (5) $-\frac{1}{2}+x,\frac{3}{2}-y,-\frac{1}{2}+z$.]

room-temperature single-crystal studies with somewhat lower precision: $Li_2[SnF_6]\cdot 2H_2O$, d(Sn—F) = 1.962–1.983 Å, mean value = 1.969 (11) Å, point-group symmetry C_{2h} (Marseglia & Brown, 1973); $Na_2[SnF_6]$, d(Sn—F) = 6 × 1.959 Å, point-group symmetry D_{2h} (Benner & Hoppe, 1990); $(Me_3NH)_2[SnF_6]\cdot 2H_2O$, d(Sn—F) = 1.932 (9)–1.965 (3) Å, mean value = 1.965 (19) Å, point group symmetry C_{2h} (Taha *et al.*, 1992). In the tetraphenylphosphonium salt $(Ph_4P)_2[SnF_6]$, the anion also exhibits point-group symmetry C_1, with Sn—F bond lengths between 1.953 (1) and 1.985 (1) Å, mean value 1.963 (14) Å, and *trans* bond angles of 179.01 (3)–178.59 (3)° (Cortijo *et al.*, 2018).

Of the six fluorine atoms, all but one (F3) also coordinate to the strontium atom. This metal atom is surrounded by five fluorine atoms and three water molecules, arranged in a distorted square-antiprismatic configuration (Fig. 1). The

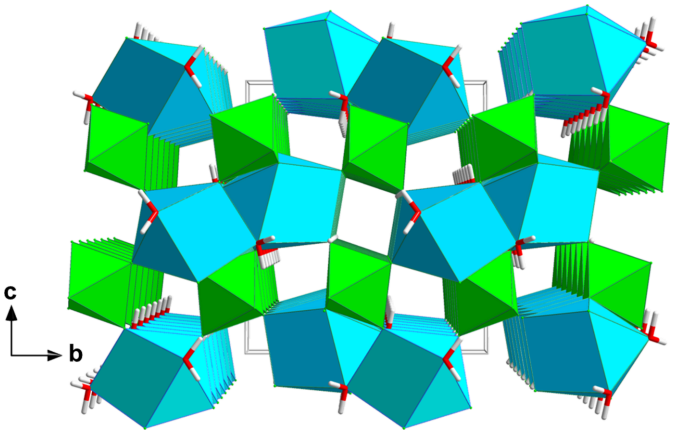


Figure 2
Polyhedral representation of the crystal packing looking down the *a* axis. $[SnF_6]^{2-}$ octahedra are drawn in green and the distorted $[SrF_5(H_2O)_3]$ square antiprisms in blue; water molecules are visualized as stick models.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H11···F3^{i}	0.96	1.92	2.796 (2)	150
O1—H12···O2^{ii}	0.96	2.06	2.986 (2)	161
O2—H21···F6^{iii}	0.96	2.50	3.263 (2)	137
O2—H22···F3^{iv}	0.96	1.81	2.764 (2)	173

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$Sr[SnF_6]\cdot 2H_2O$
M_r	356.34
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	6.0782 (4), 9.8884 (6), 11.2968 (8)
β (°)	99.154 (3)
V (Å^3)	670.33 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	11.75
Crystal size (mm)	0.29 × 0.07 × 0.07
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.458, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	73429, 1947, 1842
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.703
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.014, 0.033, 1.09
No. of reflections	1947
No. of parameters	92
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.49

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS7* (Sheldrick, 2008), *SHELXL7* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2006), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Sr—F bond lengths range from 2.4252 (14)–2.4951 (14) Å, with a mean value of 2.453 (26) Å; the strontium–oxygen bond lengths are all slightly longer, ranging from 2.6183 (17)–2.7240 (16) Å. These values can be directly compared with those of the isostructural iridium compound [ambient temperature, d(Sr—F) = 2.421 (3)–2.515 (3) Å, mean value = 2.461 (34) Å, d(Sr—O) = 2.610 (4)–2.704 (4) Å]. Three water molecules coordinate to the strontium atom, yet only two water molecules appear in the molecular formula, which is due to the fact that one water molecule (O1) bridges two strontium atoms, resulting in dimers formed by edge-sharing square antiprisms $[Sr(\mu_2\text{-}F)_5(\mu_1\text{-}H_2O)(\mu_2\text{-}H_2O)]$. Together with the octahedral $[SnF(\mu_2\text{-}F)_5]$ building blocks, the compact packing shown in Fig. 2 results.

Both water molecules are engaged in hydrogen-bonding interactions (Table 1). Based on the relatively long donor···acceptor distances (in particular for the O···O and one of the O···F contacts) and the acute bond angles at the hydrogen atoms, the hydrogen-bonding interactions are considered as medium-strong to weak.

Synthesis and crystallization

In a beaker, 0.30 g (1.56 mmol) of SnF_4 and 0.20 g (1.56 mmol) of SrF_2 were suspended in 100 ml of water, and the mixture was heated to boiling for 10 min. under stirring. The unreacted reactants were filtered off whilst hot; colorless needles of the title compound crystallized as the solution cooled and the solvent evaporated.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The four H atoms of the water molecules were clearly identified in difference-Fourier syntheses. Their positions were modeled with a common O—H distance of 0.96 Å and a H—O—H bond angle of 105.0° before they were fixed and allowed to ride on the corresponding oxygen atom with one common isotropic temperature factor.

Acknowledgements

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full crystallographic data

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Strontium hexafluoridostannate(IV) dihydrate

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Strontium hexafluoridostannate(IV) dihydrate

Crystal data

$Sr[SnF_6]\cdot 2H_2O$
M_r = 356.34
Monoclinic, $P2_1/n$
a = 6.0782 (4) Å
b = 9.8884 (6) Å
c = 11.2968 (8) Å
β = 99.154 (3)°
V = 670.33 (8) Å^3
Z = 4
$F(000)$ = 648
D_x = 3.531 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9976 reflections
θ = 2.8–30.0°
μ = 11.75 mm^{-1}
T = 100 K
Prism, colourless
0.29 × 0.07 × 0.07 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al*., 2015)
T_{min} = 0.458, T_{max} = 0.746
73429 measured reflections
1947 independent reflections
1842 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 30.0°, θ_{min} = 2.8°
h = −8→8
k = −13→13
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.014
$wR(F^2)$ = 0.033
S = 1.09
1947 reflections
92 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0112P)^2 + 1.2564P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 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	0.59421 (2)	0.53509 (2)	0.73192 (2)	0.00724 (4)
Sr1	0.66772 (3)	0.81470 (2)	0.45187 (2)	0.00759 (5)
F1	0.5712 (2)	0.64125 (15)	0.58646 (13)	0.0163 (3)
F2	0.8141 (2)	0.66012 (14)	0.81610 (13)	0.0157 (3)
F3	0.8428 (2)	0.43410 (15)	0.68662 (13)	0.0166 (3)
F4	0.6090 (2)	0.43590 (14)	0.88292 (12)	0.0151 (3)
F5	0.3769 (2)	0.40503 (14)	0.65792 (12)	0.0146 (3)
F6	0.3519 (2)	0.64425 (14)	0.77656 (12)	0.0140 (3)
O1	0.6187 (3)	1.08124 (16)	0.40924 (14)	0.0104 (3)
H11	0.5568	1.1011	0.3275	0.041 (5)*
H12	0.7467	1.1390	0.4269	0.041 (5)*
O2	1.0554 (3)	0.69766 (18)	0.51358 (16)	0.0169 (3)
H21	1.0914	0.6397	0.5821	0.041 (5)*
H22	1.1007	0.6482	0.4484	0.041 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.00757 (7)	0.00717 (7)	0.00704 (7)	0.00000 (5)	0.00136 (5)	0.00017 (5)
Sr1	0.00768 (9)	0.00759 (9)	0.00753 (9)	0.00034 (7)	0.00130 (7)	−0.00075 (7)
F1	0.0195 (7)	0.0151 (7)	0.0160 (7)	0.0028 (6)	0.0076 (5)	0.0062 (5)
F2	0.0121 (6)	0.0125 (7)	0.0208 (7)	−0.0016 (5)	−0.0023 (5)	−0.0026 (5)
F3	0.0134 (6)	0.0191 (7)	0.0173 (7)	0.0045 (5)	0.0030 (5)	−0.0043 (6)
F4	0.0151 (7)	0.0173 (7)	0.0121 (6)	−0.0004 (5)	−0.0005 (5)	0.0065 (5)
F5	0.0149 (7)	0.0125 (6)	0.0155 (7)	−0.0005 (5)	0.0000 (5)	−0.0034 (5)
F6	0.0150 (7)	0.0143 (7)	0.0139 (7)	0.0018 (5)	0.0063 (5)	−0.0012 (5)
O1	0.0086 (7)	0.0104 (7)	0.0120 (7)	−0.0006 (6)	0.0010 (6)	−0.0007 (6)
O2	0.0131 (8)	0.0187 (9)	0.0181 (9)	0.0054 (7)	0.0003 (6)	−0.0027 (7)

Geometric parameters (Å, º)

Sn1—F5	1.9356 (14)	Sr1—O1	2.6874 (16)
Sn1—F1	1.9361 (14)	Sr1—O1^{v}	2.7240 (16)
Sn1—F3	1.9464 (14)	Sr1—Sr1^{v}	4.4130 (4)
Sn1—F2	1.9530 (14)	F2—Sr1^{vi}	2.4467 (14)
Sn1—F6	1.9558 (14)	F4—Sr1^{vii}	2.4405 (13)
Sn1—F4	1.9573 (13)	F5—Sr1^{iv}	2.4951 (14)
Sr1—F1	2.4252 (14)	F6—Sr1^{viii}	2.4587 (13)
Sr1—F4^{i}	2.4405 (14)	O1—Sr1^{v}	2.7240 (16)
Sr1—F2^{ii}	2.4467 (14)	O1—H11	0.9600
Sr1—F6^{iii}	2.4587 (13)	O1—H12	0.9600
Sr1—F5^{iv}	2.4951 (14)	O2—H21	0.9600
Sr1—O2	2.6183 (17)	O2—H22	0.9600
F5—Sn1—F1	92.38 (6)	F6^{iii}—Sr1—O1	75.26 (5)

F5—Sn1—F3	92.90 (6)	F5^{iv}—Sr1—O1	139.89 (5)
F1—Sn1—F3	90.54 (6)	O2—Sr1—O1	123.41 (5)
F5—Sn1—F2	176.38 (6)	F1—Sr1—O1^{v}	70.46 (5)
F1—Sn1—F2	91.23 (6)	F4^{i}—Sr1—O1^{v}	72.70 (5)
F3—Sn1—F2	87.32 (6)	F2^{ii}—Sr1—O1^{v}	75.19 (5)
F5—Sn1—F6	89.30 (6)	F6^{iii}—Sr1—O1^{v}	144.70 (5)
F1—Sn1—F6	87.93 (6)	F5^{iv}—Sr1—O1^{v}	125.90 (5)
F3—Sn1—F6	177.37 (6)	O2—Sr1—O1^{v}	130.10 (5)
F2—Sn1—F6	90.58 (6)	O1—Sr1—O1^{v}	70.73 (6)
F5—Sn1—F4	88.68 (6)	F1—Sr1—Sr1^{v}	105.39 (3)
F1—Sn1—F4	176.81 (6)	F4^{i}—Sr1—Sr1^{v}	68.05 (3)
F3—Sn1—F4	92.41 (6)	F2^{ii}—Sr1—Sr1^{v}	71.08 (3)
F2—Sn1—F4	87.70 (6)	F6^{iii}—Sr1—Sr1^{v}	110.41 (3)
F6—Sn1—F4	89.08 (6)	F5^{iv}—Sr1—Sr1^{v}	145.86 (3)
F1—Sr1—F4^{i}	91.63 (5)	O2—Sr1—Sr1^{v}	137.13 (4)
F1—Sr1—F2^{ii}	100.89 (5)	O1—Sr1—Sr1^{v}	35.64 (3)
F4^{i}—Sr1—F2^{ii}	139.09 (5)	O1^{v}—Sr1—Sr1^{v}	35.09 (3)
F1—Sr1—F6^{iii}	143.93 (5)	Sn1—F1—Sr1	157.45 (8)
F4^{i}—Sr1—F6^{iii}	105.42 (5)	Sn1—F2—Sr1^{vi}	146.56 (7)
F2^{ii}—Sr1—F6^{iii}	86.87 (5)	Sn1—F4—Sr1^{vii}	148.80 (7)
F1—Sr1—F5^{iv}	71.21 (5)	Sn1—F5—Sr1^{iv}	143.71 (7)
F4^{i}—Sr1—F5^{iv}	144.19 (5)	Sn1—F6—Sr1^{viii}	139.19 (7)
F2^{ii}—Sr1—F5^{iv}	76.22 (5)	Sr1—O1—Sr1^{v}	109.28 (6)
F6^{iii}—Sr1—F5^{iv}	76.75 (5)	Sr1—O1—H11	112.9
F1—Sr1—O2	79.50 (5)	Sr1^{v}—O1—H11	106.7
F4^{i}—Sr1—O2	69.27 (5)	Sr1—O1—H12	118.9
F2^{ii}—Sr1—O2	151.12 (5)	Sr1^{v}—O1—H12	103.1
F6^{iii}—Sr1—O2	77.39 (5)	H11—O1—H12	105.0
F5^{iv}—Sr1—O2	76.67 (5)	Sr1—O2—H21	124.0
F1—Sr1—O1	140.80 (5)	Sr1—O2—H22	112.1
F4^{i}—Sr1—O1	71.80 (5)	H21—O2—H22	105.0
F2^{ii}—Sr1—O1	74.13 (5)		

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+3/2; (ii) *x*−1/2, −*y*+3/2, *z*−1/2; (iii) *x*+1/2, −*y*+3/2, *z*−1/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*+1, −*y*+2, −*z*+1; (vi) *x*+1/2, −*y*+3/2, *z*+1/2; (vii) −*x*+3/2, *y*−1/2, −*z*+3/2; (viii) *x*−1/2, −*y*+3/2, *z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H11···F3^{ii}	0.96	1.92	2.796 (2)	150
O1—H12···O2^{ix}	0.96	2.06	2.986 (2)	161
O2—H21···F6^{x}	0.96	2.50	3.263 (2)	137
O2—H22···F3^{xi}	0.96	1.81	2.764 (2)	173

Symmetry codes: (ii) *x*−1/2, −*y*+3/2, *z*−1/2; (ix) −*x*+2, −*y*+2, −*z*+1; (x) *x*+1, *y*, *z*; (xi) −*x*+2, −*y*+1, −*z*+1.