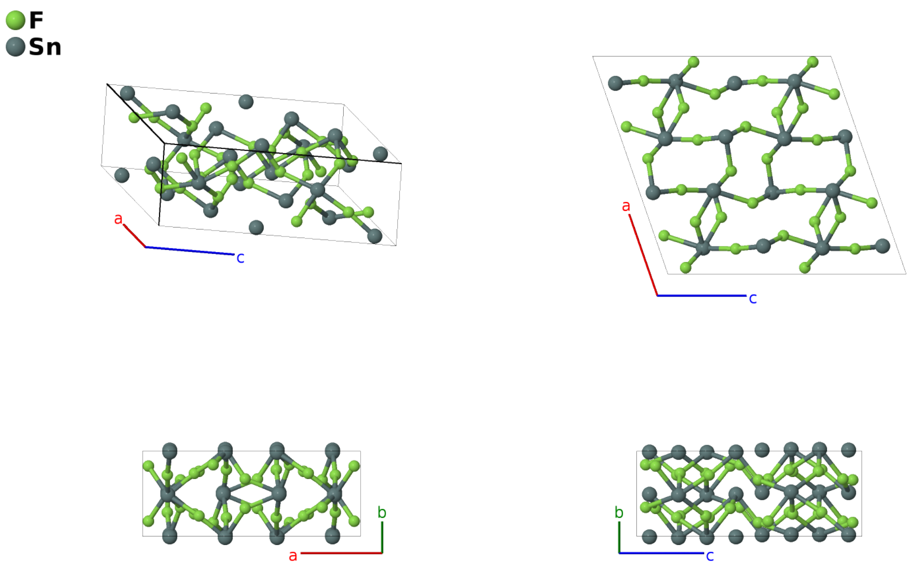
α-SnF_2 Structure: A2B_mC48_15_4f_2f-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

---

https://aflow.org/p/YKEJ

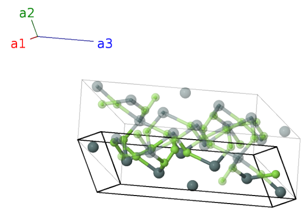
https://aflow.org/p/A2B_mC48_15_4f_2f-001



Prototype	F_2Sn
AFLOW prototype label	A2B_mC48_15_4f_2f-001
ICSD	308
Pearson symbol	mC48
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A2B_mC48_15_4f_2f-001` `--params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- SnF_2 is found in three structures:
  - monoclinic α-SnF_2 (this structure), the ground state
  - orthorhombic β-SnF_2, formed from γ-SnF_2 on cooling below 67°C, and
  - tetragonal γ-SnF_2, produced by heating α-SnF_2 above $180°C$, forming in the α-TeO_2 structure.

Base-centered Monoclinic primitive vectors



$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(x_1-y_1)\,\mathbf{a}_1+(x_1+y_1)\,\mathbf{a}_2+z_1\,\mathbf{a}_3$	=	$(ax_1+cz_1\cos\beta)\,\hat{\mathbf{x}}+by_1\,\hat{\mathbf{y}}+cz_1\sin\beta\,\hat{\mathbf{z}}$	(8f)	F I
$\mathbf{B_2}$	=	$-(x_1+y_1)\,\mathbf{a}_1-(x_1-y_1)\,\mathbf{a}_2-\left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_1+c\left(z_1-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_1\,\hat{\mathbf{y}}-c\left(z_1-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	F I
$\mathbf{B_3}$	=	$-(x_1-y_1)\,\mathbf{a}_1-(x_1+y_1)\,\mathbf{a}_2-z_1\,\mathbf{a}_3$	=	$-(ax_1+cz_1\cos\beta)\,\hat{\mathbf{x}}-by_1\,\hat{\mathbf{y}}-cz_1\sin\beta\,\hat{\mathbf{z}}$	(8f)	F I
$\mathbf{B_4}$	=	$(x_1+y_1)\,\mathbf{a}_1+(x_1-y_1)\,\mathbf{a}_2+\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_1+c\left(z_1+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_1\,\hat{\mathbf{y}}+c\left(z_1+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	F I
$\mathbf{B_5}$	=	$(x_2-y_2)\,\mathbf{a}_1+(x_2+y_2)\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$(ax_2+cz_2\cos\beta)\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}+cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B_6}$	=	$-(x_2+y_2)\,\mathbf{a}_1-(x_2-y_2)\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_2+c\left(z_2-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B_7}$	=	$-(x_2-y_2)\,\mathbf{a}_1-(x_2+y_2)\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$-(ax_2+cz_2\cos\beta)\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}-cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B_8}$	=	$(x_2+y_2)\,\mathbf{a}_1+(x_2-y_2)\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_2+c\left(z_2+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	F II
$\mathbf{B_9}$	=	$(x_3-y_3)\,\mathbf{a}_1+(x_3+y_3)\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$(ax_3+cz_3\cos\beta)\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}+cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	F III
$\mathbf{B_{10}}$	=	$-(x_3+y_3)\,\mathbf{a}_1-(x_3-y_3)\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3+c\left(z_3-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	F III
$\mathbf{B_{11}}$	=	$-(x_3-y_3)\,\mathbf{a}_1-(x_3+y_3)\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$-(ax_3+cz_3\cos\beta)\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}-cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	F III
$\mathbf{B_{12}}$	=	$(x_3+y_3)\,\mathbf{a}_1+(x_3-y_3)\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3+c\left(z_3+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	F III
$\mathbf{B_{13}}$	=	$(x_4-y_4)\,\mathbf{a}_1+(x_4+y_4)\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$(ax_4+cz_4\cos\beta)\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	F IV
$\mathbf{B_{14}}$	=	$-(x_4+y_4)\,\mathbf{a}_1-(x_4-y_4)\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4+c\left(z_4-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	F IV
$\mathbf{B_{15}}$	=	$-(x_4-y_4)\,\mathbf{a}_1-(x_4+y_4)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-(ax_4+cz_4\cos\beta)\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}-cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	F IV
$\mathbf{B_{16}}$	=	$(x_4+y_4)\,\mathbf{a}_1+(x_4-y_4)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4+c\left(z_4+\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	F IV
$\mathbf{B_{17}}$	=	$(x_5-y_5)\,\mathbf{a}_1+(x_5+y_5)\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$(ax_5+cz_5\cos\beta)\,\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}+cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	Sn I
$\mathbf{B_{18}}$	=	$-(x_5+y_5)\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5+c\left(z_5-\frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	Sn I

$\mathbf{B_{19}}$	=	$-\left(x_5 - y_5\right)\,\mathbf{a}_1 - \left(x_5 + y_5\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\left(ax_5 + cz_5\cos\beta\right)\,\mathbf{\hat{x}} - by_5\,\mathbf{\hat{y}} - cz_5\sin\beta\,\mathbf{\hat{z}}$	(8f)	Sn I
$\mathbf{B_{20}}$	=	$\left(x_5 + y_5\right)\,\mathbf{a}_1 + \left(x_5 - y_5\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Sn I
$\mathbf{B_{21}}$	=	$\left(x_6 - y_6\right)\,\mathbf{a}_1 + \left(x_6 + y_6\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\left(ax_6 + cz_6\cos\beta\right)\,\mathbf{\hat{x}} + by_6\,\mathbf{\hat{y}} + cz_6\sin\beta\,\mathbf{\hat{z}}$	(8f)	Sn II
$\mathbf{B_{22}}$	=	$-\left(x_6 + y_6\right)\,\mathbf{a}_1 - \left(x_6 - y_6\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} + by_6\,\mathbf{\hat{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Sn II
$\mathbf{B_{23}}$	=	$-\left(x_6 - y_6\right)\,\mathbf{a}_1 - \left(x_6 + y_6\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\left(ax_6 + cz_6\cos\beta\right)\,\mathbf{\hat{x}} - by_6\,\mathbf{\hat{y}} - cz_6\sin\beta\,\mathbf{\hat{z}}$	(8f)	Sn II
$\mathbf{B_{24}}$	=	$\left(x_6 + y_6\right)\,\mathbf{a}_1 + \left(x_6 - y_6\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\mathbf{\hat{x}} - by_6\,\mathbf{\hat{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\mathbf{\hat{z}}$	(8f)	Sn II

References

[1] R. C. McDonald, H. H.-K. Hau, and K. Eriks, *Crystallographic studies of tin(II) compounds. I. Crystal structure of tin(II) fluoride, SnF*$_2$, Inorg. Chem. **15**, 762–765 (1976), doi:10.1021/ic50158a003.

Found in

[1] G. Denes, J. Pannetier, and J. Lucas, *About SnF2 stannous fluoride. II. Crystal structure of* β*- and* γ*-SnF*$_2$, J. Solid State Chem. **33**, 1–11 (1980), doi:10.1016/0022-4596(80)90541-1.