

α -SnF₂ Structure:

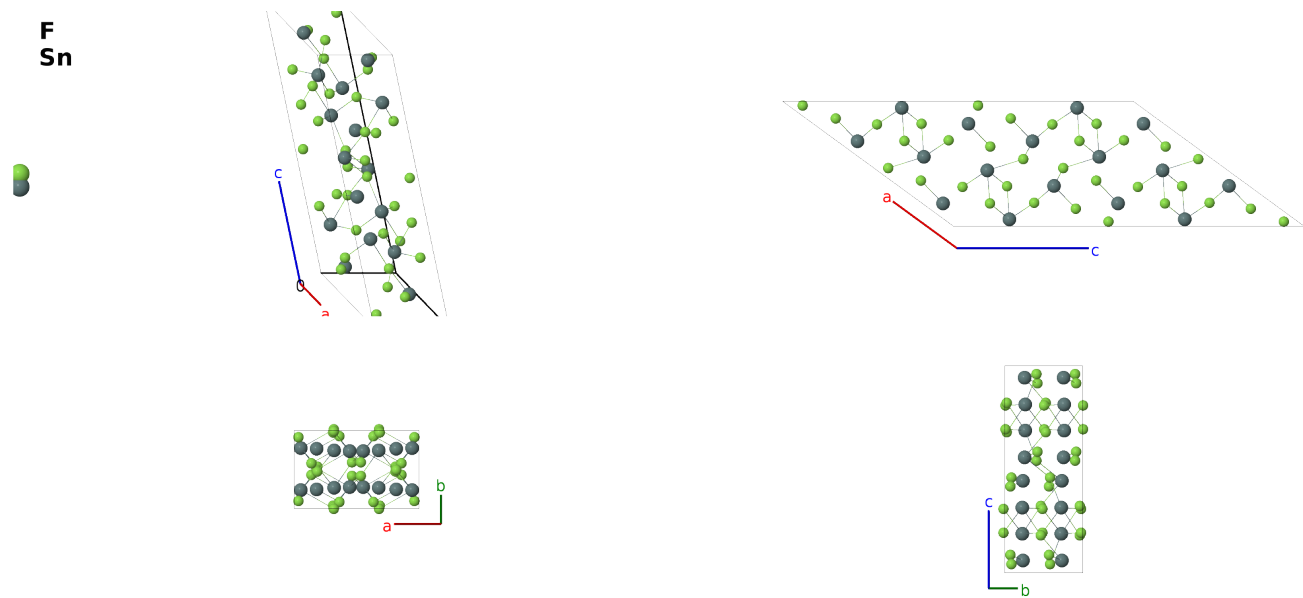
A2B_mC48_15_4f_2f-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/YKEJ>

https://aflow.org/prototype-encyclopedia/A2B_mC48_15_4f_2f-001

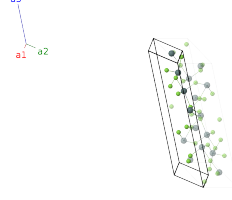


Prototype	F ₂ Sn
AFLOW prototype label	A2B_mC48_15_4f_2f-001
ICSD	308
CCDC	1590855
Pearson symbol	mC48
Space group number	15
Space group symbol	C2/c
AFLOW prototype command	<pre>aflow --proto=A2B_mC48_15_4f_2f-001 --params=a, b/a, c/a, β, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆</pre>

- SnF₂ is found in three structures:
 - monoclinic α -SnF₂ (this structure), the ground state
 - orthorhombic β -SnF₂, formed from γ -SnF₂ on cooling below 67°C, and
 - tetragonal γ -SnF₂, produced by heating α -SnF₂ above 180°C, forming in the α -TeO₂ structure.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B}_2$	$-(x_1 + y_1) \mathbf{a}_1 - (x_1 - y_1) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_1 + c(z_1 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(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
$\mathbf{B}_4$	$(x_1 + y_1) \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(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
$\mathbf{B}_6$	$-(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(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
$\mathbf{B}_8$	$(x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$-(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(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
$\mathbf{B}_{12}$	$(x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$-(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(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
$\mathbf{B}_{16}$	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$-(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Sn I

$$\mathbf{B}_{19} = \begin{matrix} -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - \\ z_5 \mathbf{a}_3 \end{matrix} = - (ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{Sn I}$$

$$\mathbf{B}_{20} = \begin{matrix} (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \\ (z_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + \\ c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Sn I}$$

$$\mathbf{B}_{21} = \begin{matrix} (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + \\ z_6 \mathbf{a}_3 \end{matrix} = (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{Sn II}$$

$$\mathbf{B}_{22} = \begin{matrix} -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - \\ (z_6 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} - (ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - \\ c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Sn II}$$

$$\mathbf{B}_{23} = \begin{matrix} -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - \\ z_6 \mathbf{a}_3 \end{matrix} = - (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{Sn II}$$

$$\mathbf{B}_{24} = \begin{matrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \\ c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Sn II}$$

References

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