

Sn₂F₃Cl Structure:

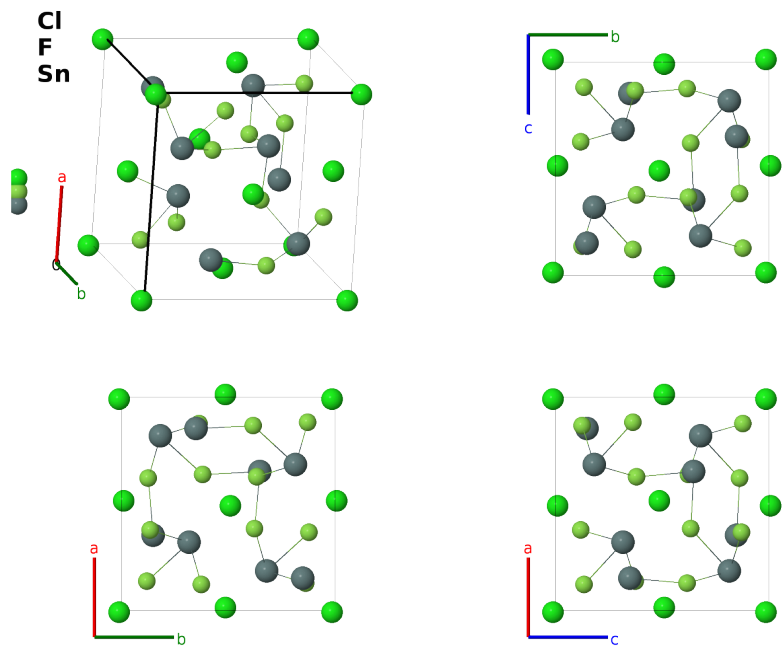
AB3C2_cP24_198_a_b_2a-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, 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/32SB>

https://aflow.org/prototype-encyclopedia/AB3C2_cP24_198_a_b_2a-001



Prototype	ClF ₃ Sn ₂
AFLOW prototype label	AB3C2_cP24_198_a_b_2a-001
ICSD	2088
CCDC	1592032
Pearson symbol	cP24
Space group number	198
Space group symbol	<i>P</i> 2 ₁ 3
AFLOW prototype command	<code>aflow --proto=AB3C2_cP24_198_a_b_2a-001</code> <code>--params=<i>a</i>, <i>x</i>₁, <i>x</i>₂, <i>x</i>₃, <i>x</i>₄, <i>y</i>₄, <i>z</i>₄</code>

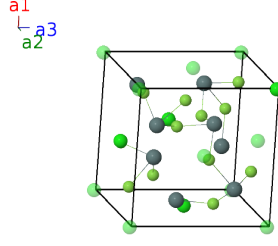
- Sn₂F₃Cl occupies the same Wyckoff positions in space group *P*2₁3 #198 as β-SnWO₄, and the ICSD assigns it to the SnWO₄ structure type. However the stoichiometry and hence the bonding are different, so we give it a separate AFLOW prototype label.

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} + a x_1 \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_1 \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} + a x_2 \hat{\mathbf{z}}$	(4a)	Sn I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Sn I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Sn I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_2 \hat{\mathbf{z}}$	(4a)	Sn I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + a x_3 \hat{\mathbf{z}}$	(4a)	Sn II
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Sn II
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Sn II
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_3 \hat{\mathbf{z}}$	(4a)	Sn II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a y_4 \hat{\mathbf{y}} + a z_4 \hat{\mathbf{z}}$	(12b)	F I
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a y_4 \hat{\mathbf{y}} + a \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	F I
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} + a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	F I
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a z_4 \hat{\mathbf{z}}$	(12b)	F I
$\mathbf{B}_{17}$	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$a z_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + a y_4 \hat{\mathbf{z}}$	(12b)	F I
$\mathbf{B}_{18}$	$= \left(z_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$a \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a y_4 \hat{\mathbf{z}}$	(12b)	F I
$\mathbf{B}_{19}$	$= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	F I
$\mathbf{B}_{20}$	$= -z_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a z_4 \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	F I
$\mathbf{B}_{21}$	$= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$a y_4 \hat{\mathbf{x}} + a z_4 \hat{\mathbf{y}} + a x_4 \hat{\mathbf{z}}$	(12b)	F I

$$\mathbf{B}_{22} = \begin{matrix} -y_4 \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 - \\ (x_4 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ay_4 \hat{\mathbf{x}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}} \quad (12b) \quad \text{F I}$$

$$\mathbf{B}_{23} = (y_4 + \frac{1}{2}) \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 - x_4 \mathbf{a}_3 = a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} \quad (12b) \quad \text{F I}$$

$$\mathbf{B}_{24} = \begin{matrix} -(y_4 - \frac{1}{2}) \mathbf{a}_1 - z_4 \mathbf{a}_2 + \\ (x_4 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}} \quad (12b) \quad \text{F I}$$

References

- [1] G. B. und L. Goost, *Kristallstruktur des Dizinn(II)-trifluorid-chlorid* **30**, 1362–1363 (1974), doi:10.1107/S0567740874004821.

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- [1] ICSD, *Inorganic Crystal Structure Database [Sn2Fe3Cl]*. ID 2088.

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