

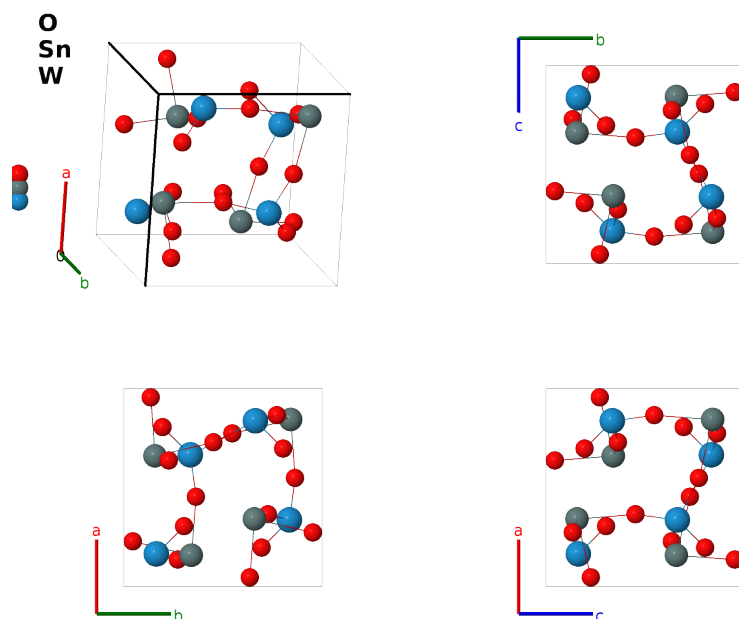
β -SnWO₄ Structure: A4BC_cP24_198_ab_a_a-001

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

https://aflow.org/prototype-encyclopedia/A4BC_cP24_198_ab_a_a-001



Prototype	O ₄ SnW
AFLOW prototype label	A4BC_cP24_198_ab_a_a-001
ICSD	2840
CCDC	1592641
Pearson symbol	cP24
Space group number	198
Space group symbol	$P2_13$
AFLOW prototype command	<code>aflow --proto=A4BC_cP24_198_ab_a_a-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>

- Below 670° this transforms into the α -SnWO₄ structure (Jeitschko, 1972).
- SnWO₄ melts above 782°C.
- The current sample was heated above 670°C and rapidly quenched.

- The atoms in $\text{Sn}_2\text{Fe}_3\text{Cl}$ occupy the same Wyckoff positions, but with different site occupations.

Simple Cubic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(4a)	Sn I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Sn I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Sn I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(4a)	Sn I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(4a)	W I
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	W I
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	W I
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(4a)	W I
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B}_{17}$	$= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B}_{18}$	$= \left(z_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B}_{19}$	$= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(12b)	O II

$$\begin{aligned}
\mathbf{B}_{20} &= -z_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -az_4 \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12b) &\quad \text{O II} \\
\mathbf{B}_{21} &= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 &= ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} &(12b) &\quad \text{O II} \\
\mathbf{B}_{22} &= -y_4 \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -ay_4 \hat{\mathbf{x}} + a \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12b) &\quad \text{O II} \\
\mathbf{B}_{23} &= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_2 - x_4 \mathbf{a}_3 &= a \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} &(12b) &\quad \text{O II} \\
\mathbf{B}_{24} &= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 - z_4 \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12b) &\quad \text{O II}
\end{aligned}$$

References

- [1] W. Jeitschko and A. W. Sleight, *Synthesis, properties and crystal structure of β -SnWO₄*, Acta Crystallogr. Sect. B **28**, 3174–3178 (1972), doi:10.1107/S056774087200768X.

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