

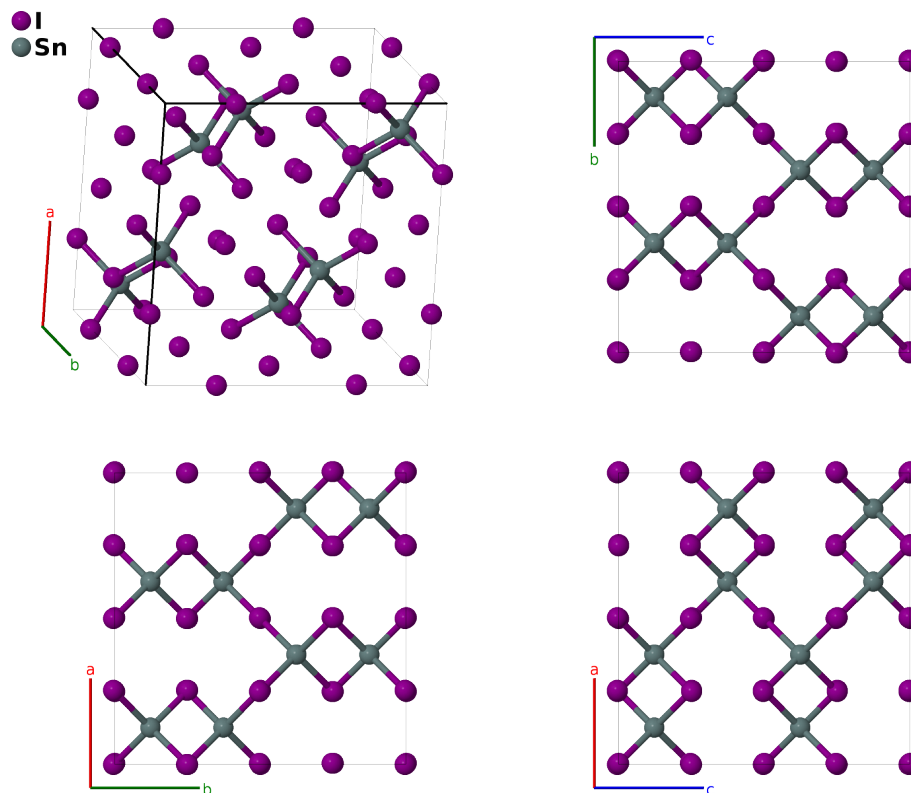
SnI₄ (D1₁) Structure: A4B_cP40_205_cd_c-001

This structure originally had the label A4B_cP40_205_cd_c. Calls to that address will be redirected here.

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<https://aflow.org/p/MJPK>

https://aflow.org/p/A4B_cP40_205_cd_c-001



Prototype	I ₄ Sn
AFLOW prototype label	A4B_cP40_205_cd_c-001
ICSD	38140
Pearson symbol	cP40
Space group number	205
Space group symbol	$Pa\bar{3}$
AFLOW prototype command	<code>aflow --proto=A4B_cP40_205_cd_c-001</code> <code>--params=a, x₁, x₂, x₃, y₃, z₃</code>

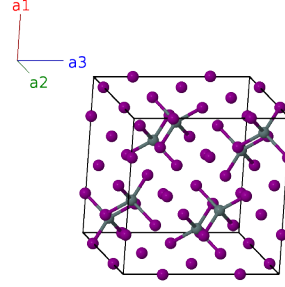
Other compounds with this structure
SiI₄, TiBr₄, TiI₄, Ni(CO)₄

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	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8c)	I I
\mathbf{B}_2	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 - x_1 \mathbf{a}_2 + (x_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	I I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 - (x_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	I I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8c)	I I
\mathbf{B}_5	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(8c)	I I
\mathbf{B}_6	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + x_1 \mathbf{a}_2 - (x_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	I I
\mathbf{B}_7	$= x_1 \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + (x_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	I I
\mathbf{B}_8	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(8c)	I I
\mathbf{B}_9	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	Sn I
\mathbf{B}_{10}	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Sn I
\mathbf{B}_{11}	$= -x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Sn I
\mathbf{B}_{12}	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	Sn I
\mathbf{B}_{13}	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(8c)	Sn I
\mathbf{B}_{14}	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 - (x_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Sn I
\mathbf{B}_{15}	$= x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + (x_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Sn I
\mathbf{B}_{16}	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(8c)	Sn I
\mathbf{B}_{17}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(24d)	I II
\mathbf{B}_{18}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	I II
\mathbf{B}_{19}	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(24d)	I II
\mathbf{B}_{20}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(24d)	I II
\mathbf{B}_{21}	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(24d)	I II
\mathbf{B}_{22}	$= (z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}}$	(24d)	I II

$$\begin{aligned}
\mathbf{B}_{23} &= \begin{matrix} -(z_3 - \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \\ (y_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{24} &= \begin{matrix} -z_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - \\ (y_3 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -az_3 \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{25} &= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3 = ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{26} &= \begin{matrix} -y_3 \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 - \\ (x_3 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ay_3 \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{27} &= (y_3 + \frac{1}{2}) \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_2 - x_3 \mathbf{a}_3 = a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{28} &= \begin{matrix} -(y_3 - \frac{1}{2}) \mathbf{a}_1 - z_3 \mathbf{a}_2 + \\ (x_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{29} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 = -ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{30} &= (x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3 = a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{31} &= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3 = ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{32} &= \begin{matrix} -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \\ z_3 \mathbf{a}_3 \end{matrix} = -a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{33} &= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3 = -az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ay_3 \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{34} &= \begin{matrix} -(z_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \\ y_3 \mathbf{a}_3 \end{matrix} = -a(z_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{35} &= (z_3 + \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 - (y_3 - \frac{1}{2}) \mathbf{a}_3 = a(z_3 + \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{36} &= z_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + (y_3 + \frac{1}{2}) \mathbf{a}_3 = az_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{37} &= -y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3 = -ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{38} &= y_3 \mathbf{a}_1 - (z_3 - \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3 = ay_3 \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{39} &= \begin{matrix} -(y_3 - \frac{1}{2}) \mathbf{a}_1 + (z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ x_3 \mathbf{a}_3 \end{matrix} = -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(z_3 + \frac{1}{2}) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (24d) & \text{I II} \\
\mathbf{B}_{40} &= (y_3 + \frac{1}{2}) \mathbf{a}_1 + z_3 \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3 = a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}} & (24d) & \text{I II}
\end{aligned}$$

References

- [1] F. Meller and I. Fankuchen, *The crystal structure of tin tetraiodide*, Acta Cryst. **8**, 343–344 (1985), doi:10.1107/S0365110X55001035.

Found in

- [1] Y. Fujii, M. Kowaka, and A. Onodera, *The pressure-induced metallic amorphous state of SnI₄. I. A novel crystal-to-amorphous transition studied by X-ray scattering*, J. Phys. C: Solid State Phys. **18**, 789–797 (1985).