

SnI₄ (D1₁) Structure: A4B_cP40_205_cd_c-001

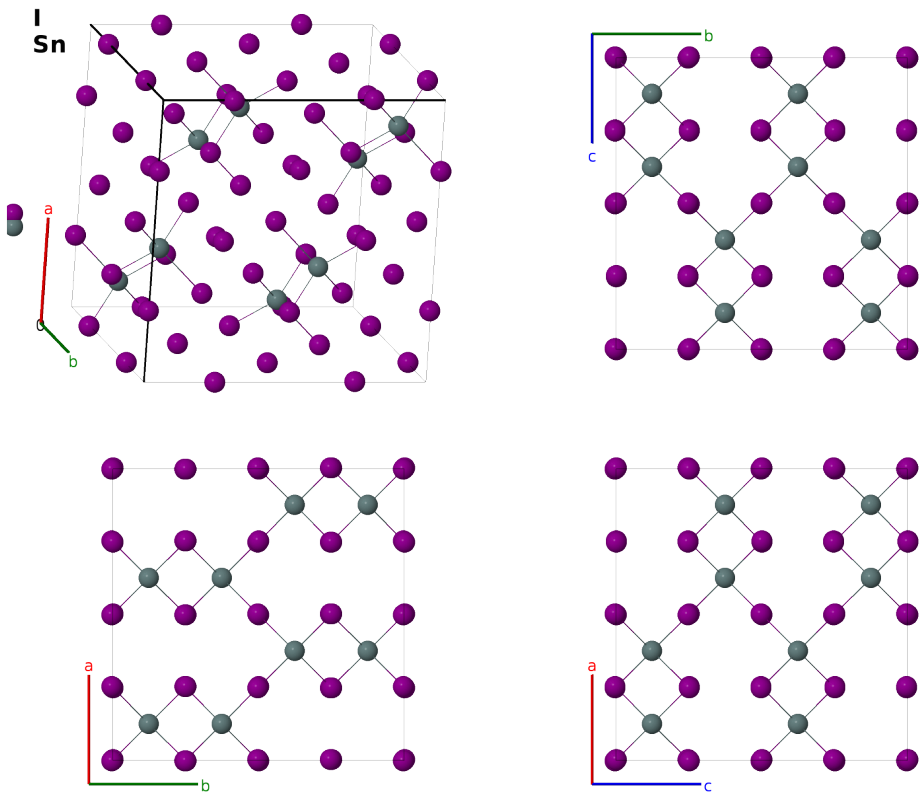
This structure previously used the label(s) **A4B_cP40_205_cd_c**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/MJPK>

https://aflow.org/prototype-encyclopedia/A4B_cP40_205_cd_c-001



Prototype	I ₄ Sn
AFLOW prototype label	A4B_cP40_205_cd_c-001
ICSD	38140
CCDC	1608859
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=$a, x_1, x_2, x_3, y_3, z_3$</code>

Other compounds with this structure

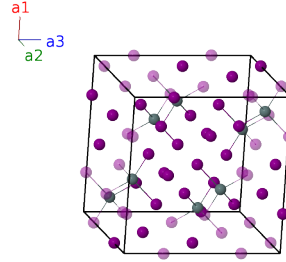
SiI₄, TiBr₄, TiI₄, Ni(CO)₄

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

$$\begin{aligned}
\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) & \text{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) & \text{I II} \\
\mathbf{B}_{23} &= -(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}_{24} &= -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}_{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} &= -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}_{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} &= -(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} \\
\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} &= -(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) & \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} &= -(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) & \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} &= -(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}_{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).

First cited in

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.