

Pt₂Sn₃ (*D*5_b) Structure: A2B3_hP10_194_f_bf-001

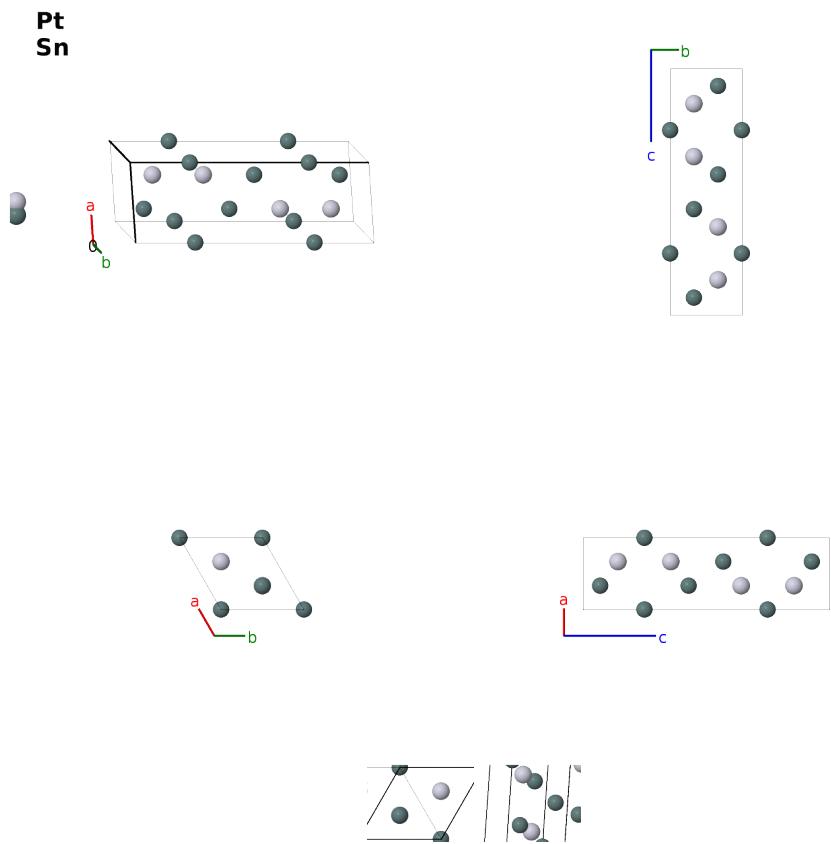
This structure previously used the label(s) **A2B3_hP10_194_f_bf**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/Y79W>

https://aflow.org/prototype-encyclopedia/A2B3_hP10_194_f_bf-001



Prototype	Pt ₂ Sn ₃
AFLOW prototype label	A2B3_hP10_194_f_bf-001
<i>Strukturbericht</i> designation	<i>D</i> 5 _b
ICSD	105794
CCDC	1663670
Pearson symbol	hP10
Space group number	194
Space group symbol	<i>P</i> 6 ₃ / <i>mmc</i>

AFLOW prototype command `aflow --proto=A2B3_hP10_194_f_bf-001`
 `--params=a, c/a, z2, z3`

Other compounds with this structure

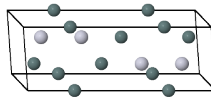
Pt₂Si₃, InAu₂Ga₂, Au₄In₃Sn₃

- We were unable to obtain a copy of (Schubert, 1949), and so we use the structural parameters given by (Pearson, 1958), using (Wood, 1947) to convert the *kX* units used by Pearson into Ångström units.
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Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$





Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(2b)	Sn I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(2b)	Sn I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4f)	Pt I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Pt I
$\mathbf{B}_5$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4f)	Pt I
$\mathbf{B}_6$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Pt I
$\mathbf{B}_7$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4f)	Sn II
$\mathbf{B}_8$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Sn II
$\mathbf{B}_9$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4f)	Sn II
$\mathbf{B}_{10}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Sn II

References

- [1] K. Schubert and H. Pfisterer, *Die Kristallstruktur von Pt₂Sn₃*, Z. Metallkd. **40**, 405 (1949).
- [2] E. A. Wood, *The Conversion Factor for kX Units to Angström Units*, J. Appl. Phys. **18**, 929 (1947), doi:10.1063/1.1697570.

Found in

- [1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 4 (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1958), 1964 reprint with corrections edn.

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