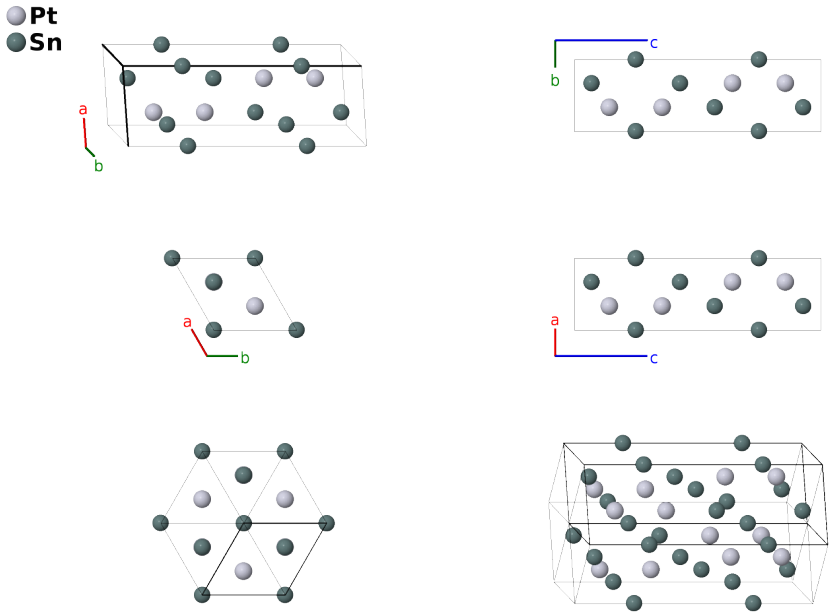
# $Pt_2Sn_3$ ($D5_b$) Structure: A2B3_hP10_194_f_bf-001

This structure originally had the label `A2B3_hP10_194_f_bf`. Calls to that address will be redirected here.

Cite this page as: 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/p/Y79W

https://aflow.org/p/A2B3_hP10_194_f_bf-001



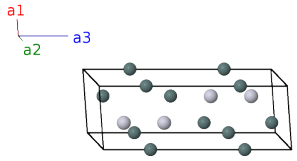

| | |
|---|---|
| **Prototype** | $Pt_2Sn_3$ |
| **AFLOW prototype label** | A2B3_hP10_194_f_bf-001 |
| ***Strukturbericht* designation** | $D5_b$ |
| **ICSD** | 105794 |
| **Pearson symbol** | hP10 |
| **Space group number** | 194 |
| **Space group symbol** | $P6_3/mmc$ |
| **AFLOW prototype command** | `aflow --proto=A2B3_hP10_194_f_bf-001 --params=`$a, c/a, z_2, z_3$ |

**Other compounds with this structure**
$Pt_2Si_3$, $InAu_2Ga_2$, $Au_4In_3Sn_3$

- 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.

## Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}} \end{aligned}$$




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\tfrac{1}{4}\,\mathbf{a}_3$ | = | $\tfrac{1}{4}c\,\hat{\mathbf{z}}$ | (2b) | Sn I |
| $\mathbf{B_2}$ | = | $\tfrac{3}{4}\,\mathbf{a}_3$ | = | $\tfrac{3}{4}c\,\hat{\mathbf{z}}$ | (2b) | Sn I |
| $\mathbf{B_3}$ | = | $\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4f) | Pt I |
| $\mathbf{B_4}$ | = | $\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \tfrac{1}{2}\right)\,\mathbf{a}_3$ | = | $\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4f) | Pt I |
| $\mathbf{B_5}$ | = | $\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (4f) | Pt I |
| $\mathbf{B_6}$ | = | $\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 - \left(z_2 - \tfrac{1}{2}\right)\,\mathbf{a}_3$ | = | $\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4f) | Pt I |
| $\mathbf{B_7}$ | = | $\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (4f) | Sn II |
| $\mathbf{B_8}$ | = | $\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 + \left(z_3 + \tfrac{1}{2}\right)\,\mathbf{a}_3$ | = | $\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4f) | Sn II |
| $\mathbf{B_9}$ | = | $\tfrac{2}{3}\,\mathbf{a}_1 + \tfrac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (4f) | Sn II |
| $\mathbf{B_{10}}$ | = | $\tfrac{1}{3}\,\mathbf{a}_1 + \tfrac{2}{3}\,\mathbf{a}_2 - \left(z_3 - \tfrac{1}{2}\right)\,\mathbf{a}_3$ | = | $\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4f) | Sn II |

## References


[1] K. Schubert and H. Pfisterer, *Die Kristallstruktur von $Pt_2Sn_3$*, 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, Frankfort, 1958), 1964 reprint with corrections edn.