Sn_4P_3 Structure: A3B4_hR7_166_ac_2c-002

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/W0LQ

https://aflow.org/prototype-encyclopedia/A3B4_hR7_166_ac_2c-002

Prototype	P_3Sn_4
AFLOW prototype label	A3B4_hR7_166_ac_2c-002
ICSD	15014
CCDC	1595799
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B4_hR7_166_ac_2c-002 --params=`$a, c/a, x_2, x_3, x_4$

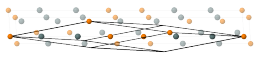
Other compounds with this structure

Se_4Bi_3 (poubaite), Bi_4Se_3 (laitakarite), Bi_4Te_4, Sn_4As_3

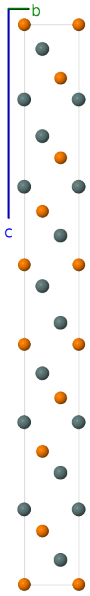
- The Sn-P phase diagram has three known phases (Zavrazhnova, 2018):
  - SnP_3
  - Sn_4P_3 (this structure)
  - Sn_3P_4
- Sn_4P_3 is the binary form of $GeSb_2Te_4$.
- In_3Te_4 and Sn_4P_3 have the same AFLOW prototype label, A3B4_hR7_166_ac_2c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

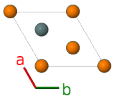
Rhombohedral primitive vectors

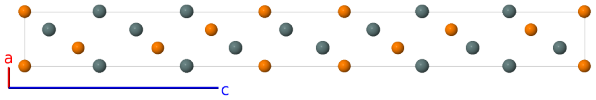
$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$

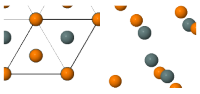


P
Sn









Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	P I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	P II
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	P II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Sn I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Sn I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Sn II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Sn II

References

[1] O. Olofsson, *X-Ray Investigation of the Tin-Phosphorus System*, Acta Chem. Scand. **24**, 1153–1162 (1970), doi:10.3891/acta.chem.scand.24-1153.

[2] A. Y. Zavrazhnova, V. Semenova, E. Y. Proskurina, and T. P. Sushkova, *Phase diagram of the Sn-P system*, J. Therm. Anal. Calorim. **134**, 475–481 (2018), doi:10.1007/s10973-018-7123-0.

Found in

[1] Q. Liu, P.-J. Guo, S. Xu, X.-Y. Yue, H. Wang, X.-Y. Wang, H. Liang, D.-D. Wu, Y. Sun, Q.-J. Li, T.-L. Xia, X.-F. Sun, and Y.-Y. Wang, *Quantum Oscillation and Electronic Structure of Sn_4As_3 and Sn_4P_3*, J. Phys. Chem. C **127**, 4319–4325 (2023), doi:10.1021/acs.jpcc.2c08206.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).