

Sn₃P₄ Structure:

A16B3_hR19_166_2c2h_ac-001

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<https://aflow.org/prototype-encyclopedia/17E5>

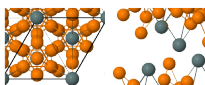
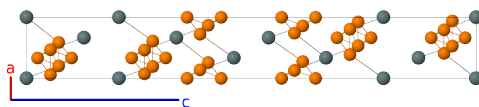
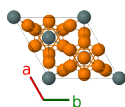
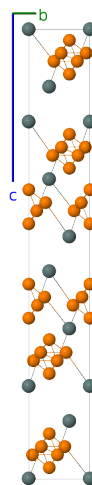
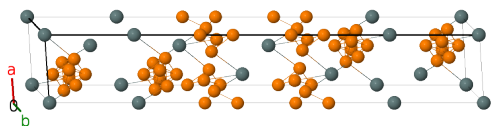
https://aflow.org/prototype-encyclopedia/A16B3_hR19_166_2c2h_ac-001

Prototype	P ₄ Sn ₃
AFLOW prototype label	A16B3_hR19_166_2c2h_ac-001
ICSD	159922
CCDC	1676344
Pearson symbol	hR19
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A16B3_hR19_166_2c2h_ac-001</code> <code>--params=$a, c/a, x_2, x_3, x_4, x_5, z_5, x_6, z_6$</code>

- The Sn-P phase diagram has three known phases (Zavrazhnova, 2018):
 - SnP₃
 - Sn₄P₃
 - Sn₃P₄ (this structure)
- While the tin sites are fully occupied, the phosphorous sites of Sn₃P₄ are highly disordered:
 - The P I (2c) site is 24% occupied.
 - The P II (2c) site is 22.2% occupied.
 - The P III (6h) site is 26.1% occupied.
 - The P IV (6h) site is 25.6% occupied.
- These partial occupations give the observed stoichiometry.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

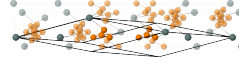
Rhombohedral primitive vectors

P
Sn





$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) Sn 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 I
$\mathbf{B}_3$	=	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$-cx_2 \hat{\mathbf{z}}$	(2c) P I
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$cx_3 \hat{\mathbf{z}}$	(2c) P II
$\mathbf{B}_5$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-cx_3 \hat{\mathbf{z}}$	(2c) P II
$\mathbf{B}_6$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$cx_4 \hat{\mathbf{z}}$	(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
$\mathbf{B}_8$	=	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h) P III
$\mathbf{B}_9$	=	$z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h) P III
$\mathbf{B}_{10}$	=	$x_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h) P III
$\mathbf{B}_{11}$	=	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h) P III
$\mathbf{B}_{12}$	=	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h) P III
$\mathbf{B}_{13}$	=	$-x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a(x_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(2x_5 + z_5) \hat{\mathbf{z}}$	(6h) P III
$\mathbf{B}_{14}$	=	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h) P IV
$\mathbf{B}_{15}$	=	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h) P IV
$\mathbf{B}_{16}$	=	$x_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h) P IV
$\mathbf{B}_{17}$	=	$-z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	=	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h) P IV
$\mathbf{B}_{18}$	=	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h) P IV
$\mathbf{B}_{19}$	=	$-x_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a(x_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(2x_6 + z_6) \hat{\mathbf{z}}$	(6h) P IV

References

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- [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.

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