SnP_3 Structure: A3B_hR8_166_h_c-001

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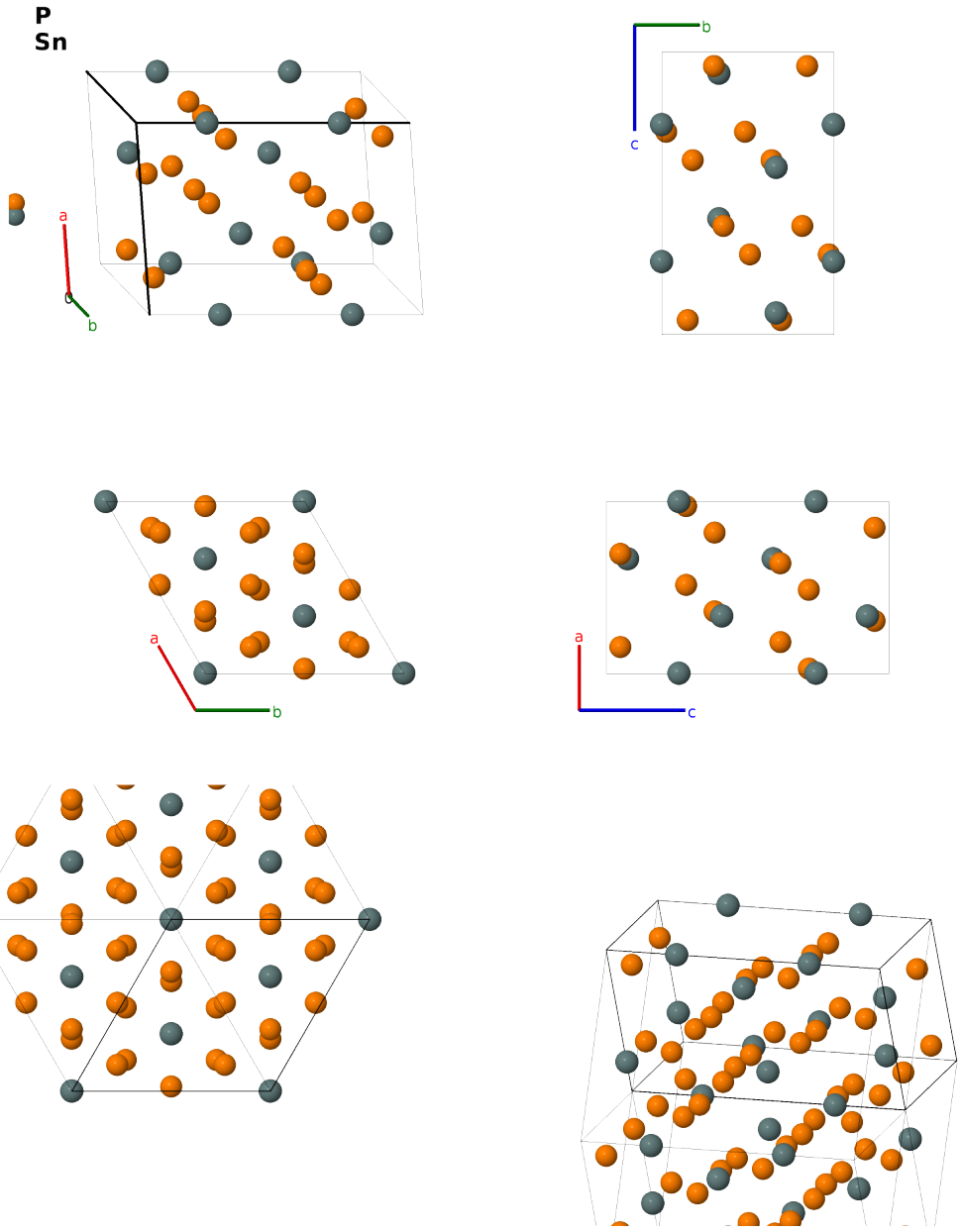
https://aflow.org/prototype-encyclopedia/JF25

https://aflow.org/prototype-encyclopedia/A3B_hR8_166_h_c-001



Prototype	P_3Sn
AFLOW prototype label	A3B_hR8_166_h_c-001

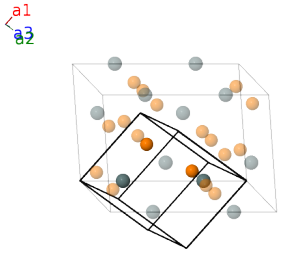
ICSD	16293
CCDC	1596892
Pearson symbol	hR8
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B_hR8_166_h_c-001 --params=`$a, c/a, x_1, x_2, z_2$

Other compounds with this structure
GeP_3

- The Sn-P phase diagram has three known phases (Zavrazhnova, 2018):
  - SnP_3 (this structure)
  - Sn_4P_3
  - Sn_3P_4
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	Sn I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	Sn I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_4}$	=	$z_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_2 - z_2)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_6}$	=	$-z_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 - z_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	P I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_2 - z_2)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_2 + z_2)\,\hat{\mathbf{z}}$	(6h)	P I

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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