Sn_4As_3 Structure: A3B4_hR7_160_3a_4a-001

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https://aflow.org/p/RN9C

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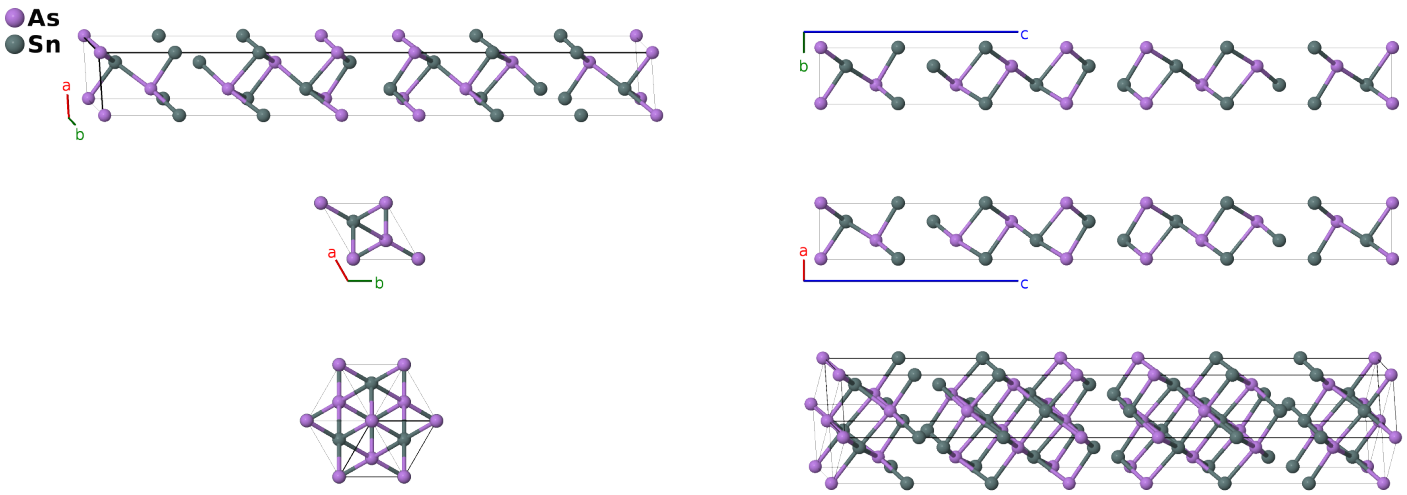
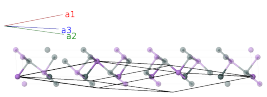


Prototype	As_3Sn_4
AFLOW prototype label	A3B4_hR7_160_3a_4a-001
ICSD	419884
Pearson symbol	hR7
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=A3B4_hR7_160_3a_4a-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, x_6, x_7$

- Most earlier *e.g.* (Pearson, 1967) work places this in space group $R\bar{3}m$ #166, in which case this would be in the Al_4C_3 ($D7_1$) structure. (Kovnir, 2009) argue that there is actually no inversion site, so the structure is as presented here, in space group $R3m$ #160. The two structures are very close – if we allow a 0.1Å uncertainty in the atomic positions the structure becomes $D7_1$. As we already have that structure, we present the Kovnir *et al.* structure here.
- 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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	As I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	As II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(1a)	As III
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(1a)	Sn I
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$cx_5\,\hat{\mathbf{z}}$	(1a)	Sn II
$\mathbf{B_6}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$cx_6\,\hat{\mathbf{z}}$	(1a)	Sn III
$\mathbf{B_7}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$cx_7\,\hat{\mathbf{z}}$	(1a)	Sn IV

References

[1] K. Kovnir, Y. V. Kolen'ko, A. I. Baranov, I. S. Neira, A. V. Sobolev, M. Yoshimura, I. A. .Presniakov, and A. V. Shevelkov, *Sn_4As_3 revisited: Solvothermal synthesis and crystal and electronic structure*, J. Solid State Chem. **182**, 630–639 (2009), doi:10.1016/j.jssc.2008.12.007.

[2] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).