

Sn₄As₃ Structure:

A3B4_hR7_160_3a_4a-001

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<https://aflow.org/prototype-encyclopedia/RN9C>

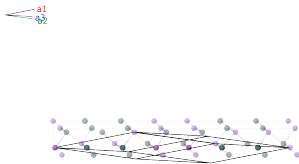
https://aflow.org/prototype-encyclopedia/A3B4_hR7_160_3a_4a-001

Prototype	As ₃ Sn ₄
AFLOW prototype label	A3B4_hR7_160_3a_4a-001
ICSD	419884
CCDC	1732469
Pearson symbol	hR7
Space group number	160
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A3B4_hR7_160_3a_4a-001</code> <code>--params=a, c/a, x₁, x₂, x₃, x₄, x₅, x₆, x₇</code>

- 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 Al₄C₃ ($D7_1$) structure. (Kovnir, 2009) argue that there is actually no inversion site, so the structure is as presented here, in space group $R\bar{3}m$ #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

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



Basis vectors

Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
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$\mathbf{B}_1$	=	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$cx_1 \hat{\mathbf{z}}$	(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, *Sn₄As₃ 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).

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Sn

