

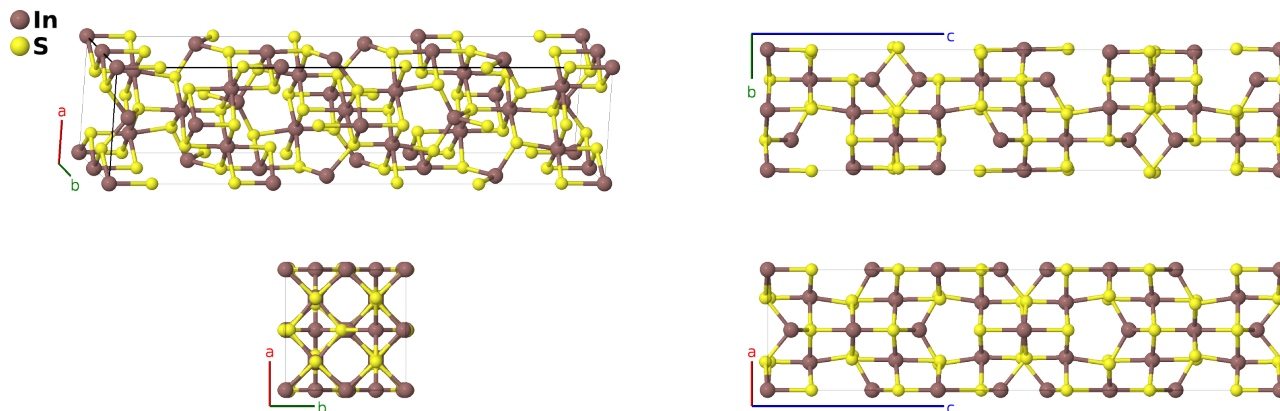
β -In₂S₃ Structure: A2B3_tI80_141_ceh_3h-001

This structure originally had the label **A2B3_tI80_141_ceh_3h**. Calls to that address will be redirected here.

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<https://aflow.org/p/PJGC>

https://aflow.org/p/A2B3_tI80_141_ceh_3h-001



Prototype	In ₂ S ₃
AFLOW prototype label	A2B3_tI80_141_ceh_3h-001
ICSD	151644
Pearson symbol	tI80
Space group number	141
Space group symbol	<i>I</i> 4 ₁ / <i>amd</i>
AFLOW prototype command	<code>aflow --proto=A2B3_tI80_141_ceh_3h-001 --params=a, c/a, z₂, y₃, z₃, y₄, z₄, y₅, z₅, y₆, z₆</code>

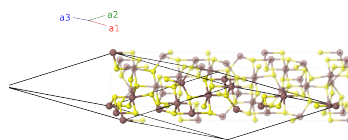
- This is a spinel structure with ordered defects.

Body-centered Tetragonal primitive vectors

$$\mathbf{a}_1 = -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(8c) In I

$$\mathbf{B}_{36} = z_6 \mathbf{a}_1 + (y_6 + z_6) \mathbf{a}_2 + (y_6 + \frac{1}{2}) \mathbf{a}_3 = a (y_6 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_6 - \frac{1}{4}) \hat{\mathbf{z}} \quad (16h) \quad \text{S III}$$

$$\mathbf{B}_{37} = (y_6 - z_6 + \frac{1}{2}) \mathbf{a}_1 - z_6 \mathbf{a}_2 + (y_6 + \frac{1}{2}) \mathbf{a}_3 = a (y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} \quad (16h) \quad \text{S III}$$

$$\mathbf{B}_{38} = -(y_6 + z_6) \mathbf{a}_1 - z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 = -ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} \quad (16h) \quad \text{S III}$$

$$\mathbf{B}_{39} = -z_6 \mathbf{a}_1 + (y_6 - z_6 + \frac{1}{2}) \mathbf{a}_2 + y_6 \mathbf{a}_3 = a (y_6 + \frac{1}{4}) \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} - c (z_6 - \frac{1}{4}) \hat{\mathbf{z}} \quad (16h) \quad \text{S III}$$

$$\mathbf{B}_{40} = -z_6 \mathbf{a}_1 - (y_6 + z_6) \mathbf{a}_2 - (y_6 - \frac{1}{2}) \mathbf{a}_3 = -a (y_6 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - c (z_6 + \frac{1}{4}) \hat{\mathbf{z}} \quad (16h) \quad \text{S III}$$

References

- [1] N. S. Rampersadh, A. M. Venter, and D. G. Billing, *Rietveld refinement of In_2S_3 using neutron and X-ray powder diffraction data*, Physica B **350**, e383–e385 (2004), doi:10.1016/j.physb.2004.03.102.