β-In_2S_3 Structure: A2B3_tI80_141_ceh_3h-001

This structure previously used the label(s) `A2B3_tI80_141_ceh_3h`. Calls to these addresses will be redirected here.

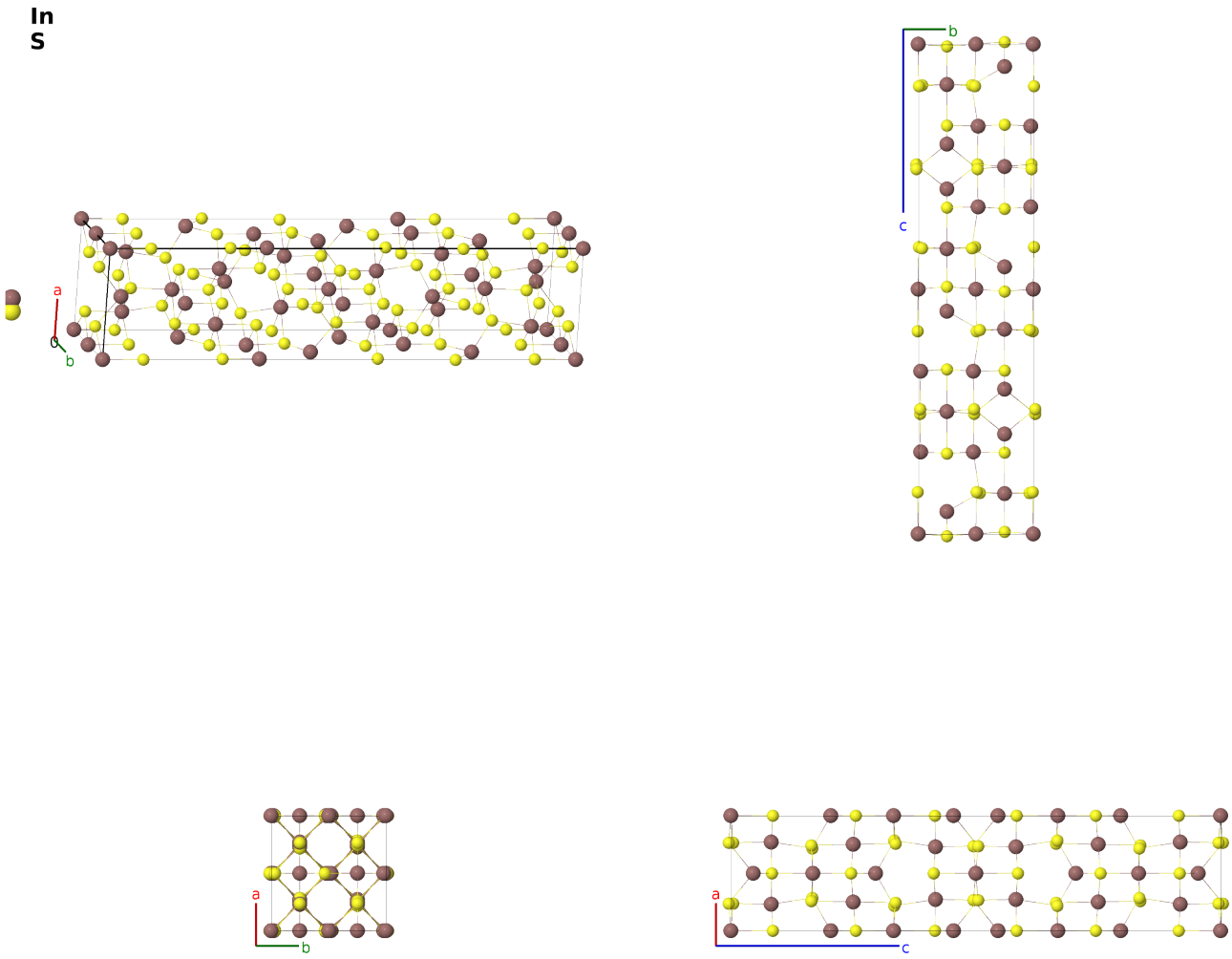
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

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

https://aflow.org/prototype-encyclopedia/A2B3_tI80_141_ceh_3h-001



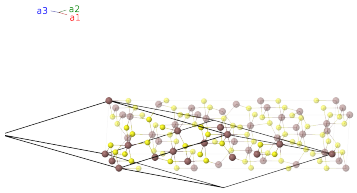
Prototype In_2S_3

AFLOW prototype label	A2B3_tI80_141_ceh_3h-001
ICSD	151644
CCDC	1668469
Pearson symbol	tI80
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A2B3_tI80_141_ceh_3h-001 --params=`$a, c/a, z_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6$

- This is a spinel structure with ordered defects.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(8c)	In I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(8c)	In I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	In I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	In I
$\mathbf{B_5}$	=	$\left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8e)	In II
$\mathbf{B_6}$	=	$z_2\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	In II
$\mathbf{B_7}$	=	$-\left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8e)	In II
$\mathbf{B_8}$	=	$-z_2\,\mathbf{a}_1 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8e)	In II
$\mathbf{B_9}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B_{10}}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B_{11}}$	=	$z_3\,\mathbf{a}_1 + \left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B_{12}}$	=	$z_3\,\mathbf{a}_1 + (y_3 + z_3)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B_{13}}$	=	$\left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B_{14}}$	=	$-(y_3 + z_3)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16h)	In III

$\mathbf{B_{15}}$	=	$-z_3\,\mathbf{a}_1+\left(y_3-z_3+\frac{1}{2}\right)\,\mathbf{a}_2+y_3\,\mathbf{a}_3$	=	$a\left(y_3+\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B_{16}}$	=	$-z_3\,\mathbf{a}_1-\left(y_3+z_3\right)\,\mathbf{a}_2-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B_{17}}$	=	$\left(y_4+z_4\right)\,\mathbf{a}_1+z_4\,\mathbf{a}_2+y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B_{18}}$	=	$\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_1+z_4\,\mathbf{a}_2-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B_{19}}$	=	$z_4\,\mathbf{a}_1+\left(-y_4+z_4+\frac{1}{2}\right)\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B_{20}}$	=	$z_4\,\mathbf{a}_1+\left(y_4+z_4\right)\,\mathbf{a}_2+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B_{21}}$	=	$\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B_{22}}$	=	$-\left(y_4+z_4\right)\,\mathbf{a}_1-z_4\,\mathbf{a}_2-y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B_{23}}$	=	$-z_4\,\mathbf{a}_1+\left(y_4-z_4+\frac{1}{2}\right)\,\mathbf{a}_2+y_4\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B_{24}}$	=	$-z_4\,\mathbf{a}_1-\left(y_4+z_4\right)\,\mathbf{a}_2-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_4+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B_{25}}$	=	$\left(y_5+z_5\right)\,\mathbf{a}_1+z_5\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B_{26}}$	=	$\left(-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1+z_5\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B_{27}}$	=	$z_5\,\mathbf{a}_1+\left(-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B_{28}}$	=	$z_5\,\mathbf{a}_1+\left(y_5+z_5\right)\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B_{29}}$	=	$\left(y_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B_{30}}$	=	$-\left(y_5+z_5\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B_{31}}$	=	$-z_5\,\mathbf{a}_1+\left(y_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B_{32}}$	=	$-z_5\,\mathbf{a}_1-\left(y_5+z_5\right)\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_5+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B_{33}}$	=	$\left(y_6+z_6\right)\,\mathbf{a}_1+z_6\,\mathbf{a}_2+y_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(16h)	S III
$\mathbf{B_{34}}$	=	$\left(-y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_1+z_6\,\mathbf{a}_2-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(16h)	S III
$\mathbf{B_{35}}$	=	$z_6\,\mathbf{a}_1+\left(-y_6+z_6+\frac{1}{2}\right)\,\mathbf{a}_2-y_6\,\mathbf{a}_3$	=	$-a\left(y_6-\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S III
$\mathbf{B_{36}}$	=	$z_6\,\mathbf{a}_1+\left(y_6+z_6\right)\,\mathbf{a}_2+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_6+\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_6-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S III
$\mathbf{B_{37}}$	=	$\left(y_6-z_6+\frac{1}{2}\right)\,\mathbf{a}_1-z_6\,\mathbf{a}_2+\left(y_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(16h)	S III
$\mathbf{B_{38}}$	=	$-\left(y_6+z_6\right)\,\mathbf{a}_1-z_6\,\mathbf{a}_2-y_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{y}}-cz_6\,\hat{\mathbf{z}}$	(16h)	S III
$\mathbf{B_{39}}$	=	$-z_6\,\mathbf{a}_1+\left(y_6-z_6+\frac{1}{2}\right)\,\mathbf{a}_2+y_6\,\mathbf{a}_3$	=	$a\left(y_6+\frac{1}{4}\right)\,\hat{\mathbf{x}}-\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_6-\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	S III
$\mathbf{B_{40}}$	=	$-z_6\,\mathbf{a}_1-\left(y_6+z_6\right)\,\mathbf{a}_2-\left(y_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_6-\frac{1}{4}\right)\,\hat{\mathbf{x}}+\frac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_6+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017