

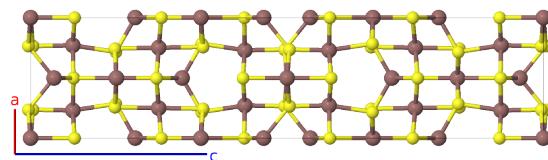
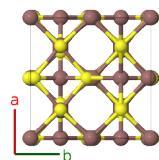
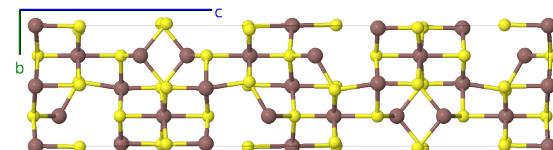
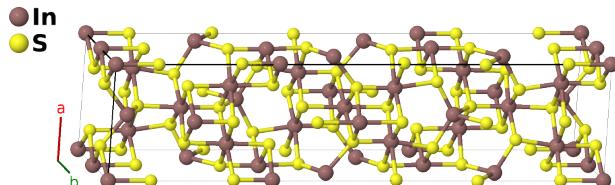
# $\beta$ -In<sub>2</sub>S<sub>3</sub> Structure: A2B3\_tI80\_141\_ceh\_3h-001

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](https://aflow.org/p/A2B3_tI80_141_ceh_3h-001)

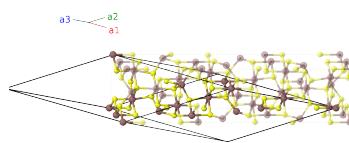


Prototype	In <sub>2</sub> S <sub>3</sub>
AFLOW prototype label	A2B3_tI80_141_ceh_3h-001
ICSD	151644
Pearson symbol	tI80
Space group number	141
Space group symbol	<i>I</i> 4 <sub>1</sub> / <i>amd</i>
AFLOW prototype command	aflow --proto=A2B3_tI80_141_ceh_3h-001 --params= <i>a</i> , <i>c/a</i> , <i>z</i> <sub>2</sub> , <i>y</i> <sub>3</sub> , <i>z</i> <sub>3</sub> , <i>y</i> <sub>4</sub> , <i>z</i> <sub>4</sub> , <i>y</i> <sub>5</sub> , <i>z</i> <sub>5</sub> , <i>y</i> <sub>6</sub> , <i>z</i> <sub>6</sub>

- This is a spinel structure with ordered defects.

## Body-centered Tetragonal primitive vectors

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



## 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
$\mathbf{B}_5$	$=$	$(z_2 + \frac{1}{4})\mathbf{a}_1 + z_2\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(8e)	In II
$\mathbf{B}_6$	$=$	$z_2\mathbf{a}_1 + (z_2 + \frac{1}{4})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + c(z_2 - \frac{1}{4})\hat{\mathbf{z}}$	(8e)	In II
$\mathbf{B}_7$	$=$	$-(z_2 - \frac{3}{4})\mathbf{a}_1 - z_2\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(8e)	In II
$\mathbf{B}_8$	$=$	$-z_2\mathbf{a}_1 - (z_2 - \frac{3}{4})\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} - c(z_2 - \frac{1}{4})\hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$=$	$(-y_3 + z_3 + \frac{1}{2})\mathbf{a}_1 + z_3\mathbf{a}_2 - (y_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_3 - \frac{1}{2})\hat{\mathbf{y}} + cz_3\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B}_{11}$	$=$	$z_3\mathbf{a}_1 + (-y_3 + z_3 + \frac{1}{2})\mathbf{a}_2 - y_3\mathbf{a}_3$	$=$	$-a(y_3 - \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + c(z_3 + \frac{1}{4})\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B}_{12}$	$=$	$z_3\mathbf{a}_1 + (y_3 + z_3)\mathbf{a}_2 + (y_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + c(z_3 - \frac{1}{4})\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B}_{13}$	$=$	$(y_3 - z_3 + \frac{1}{2})\mathbf{a}_1 - z_3\mathbf{a}_2 + (y_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{2})\hat{\mathbf{y}} - cz_3\hat{\mathbf{z}}$	(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
$\mathbf{B}_{15}$	$=$	$-z_3\mathbf{a}_1 + (y_3 - z_3 + \frac{1}{2})\mathbf{a}_2 + y_3\mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} - c(z_3 - \frac{1}{4})\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B}_{16}$	$=$	$-z_3\mathbf{a}_1 - (y_3 + z_3)\mathbf{a}_2 - (y_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_3 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - c(z_3 + \frac{1}{4})\hat{\mathbf{z}}$	(16h)	In III
$\mathbf{B}_{17}$	$=$	$(y_4 + z_4)\mathbf{a}_1 + z_4\mathbf{a}_2 + y_4\mathbf{a}_3$	$=$	$ay_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B}_{18}$	$=$	$(-y_4 + z_4 + \frac{1}{2})\mathbf{a}_1 + z_4\mathbf{a}_2 - (y_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2})\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B}_{19}$	$=$	$z_4\mathbf{a}_1 + (-y_4 + z_4 + \frac{1}{2})\mathbf{a}_2 - y_4\mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + c(z_4 + \frac{1}{4})\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B}_{20}$	$=$	$z_4\mathbf{a}_1 + (y_4 + z_4)\mathbf{a}_2 + (y_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + c(z_4 - \frac{1}{4})\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B}_{21}$	$=$	$(y_4 - z_4 + \frac{1}{2})\mathbf{a}_1 - z_4\mathbf{a}_2 + (y_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2})\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B}_{22}$	$=$	$-(y_4 + z_4)\mathbf{a}_1 - z_4\mathbf{a}_2 - y_4\mathbf{a}_3$	$=$	$-ay_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B}_{23}$	$=$	$-z_4\mathbf{a}_1 + (y_4 - z_4 + \frac{1}{2})\mathbf{a}_2 + y_4\mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} - c(z_4 - \frac{1}{4})\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B}_{24}$	$=$	$-z_4\mathbf{a}_1 - (y_4 + z_4)\mathbf{a}_2 - (y_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - c(z_4 + \frac{1}{4})\hat{\mathbf{z}}$	(16h)	S I
$\mathbf{B}_{25}$	$=$	$(y_5 + z_5)\mathbf{a}_1 + z_5\mathbf{a}_2 + y_5\mathbf{a}_3$	$=$	$ay_5\hat{\mathbf{y}} + cz_5\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B}_{26}$	$=$	$(-y_5 + z_5 + \frac{1}{2})\mathbf{a}_1 + z_5\mathbf{a}_2 - (y_5 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_5 - \frac{1}{2})\hat{\mathbf{y}} + cz_5\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B}_{27}$	$=$	$z_5\mathbf{a}_1 + (-y_5 + z_5 + \frac{1}{2})\mathbf{a}_2 - y_5\mathbf{a}_3$	$=$	$-a(y_5 - \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + c(z_5 + \frac{1}{4})\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B}_{28}$	$=$	$z_5\mathbf{a}_1 + (y_5 + z_5)\mathbf{a}_2 + (y_5 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + c(z_5 - \frac{1}{4})\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B}_{29}$	$=$	$(y_5 - z_5 + \frac{1}{2})\mathbf{a}_1 - z_5\mathbf{a}_2 + (y_5 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2})\hat{\mathbf{y}} - cz_5\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B}_{30}$	$=$	$-(y_5 + z_5)\mathbf{a}_1 - z_5\mathbf{a}_2 - y_5\mathbf{a}_3$	$=$	$-ay_5\hat{\mathbf{y}} - cz_5\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B}_{31}$	$=$	$-z_5\mathbf{a}_1 + (y_5 - z_5 + \frac{1}{2})\mathbf{a}_2 + y_5\mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} - c(z_5 - \frac{1}{4})\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B}_{32}$	$=$	$-z_5\mathbf{a}_1 - (y_5 + z_5)\mathbf{a}_2 - (y_5 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_5 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - c(z_5 + \frac{1}{4})\hat{\mathbf{z}}$	(16h)	S II
$\mathbf{B}_{33}$	$=$	$(y_6 + z_6)\mathbf{a}_1 + z_6\mathbf{a}_2 + y_6\mathbf{a}_3$	$=$	$ay_6\hat{\mathbf{y}} + cz_6\hat{\mathbf{z}}$	(16h)	S III
$\mathbf{B}_{34}$	$=$	$(-y_6 + z_6 + \frac{1}{2})\mathbf{a}_1 + z_6\mathbf{a}_2 - (y_6 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2})\hat{\mathbf{y}} + cz_6\hat{\mathbf{z}}$	(16h)	S III
$\mathbf{B}_{35}$	$=$	$z_6\mathbf{a}_1 + (-y_6 + z_6 + \frac{1}{2})\mathbf{a}_2 - y_6\mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{4}a\hat{\mathbf{y}} + c(z_6 + \frac{1}{4})\hat{\mathbf{z}}$	(16h)	S III

$$\begin{aligned}
\mathbf{B}_{36} &= z_6 \mathbf{a}_1 + (y_6 + z_6) \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 & = & a \left(y_6 + \frac{1}{4}\right) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + c \left(z_6 - \frac{1}{4}\right) \hat{\mathbf{z}} & (16h) & S III \\
\mathbf{B}_{37} &= \left(y_6 - z_6 + \frac{1}{2}\right) \mathbf{a}_1 - z_6 \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 & = & a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16h) & S III \\
\mathbf{B}_{38} &= -(y_6 + z_6) \mathbf{a}_1 - z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 & = & -ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16h) & S III \\
\mathbf{B}_{39} &= -z_6 \mathbf{a}_1 + \left(y_6 - z_6 + \frac{1}{2}\right) \mathbf{a}_2 + y_6 \mathbf{a}_3 & = & a \left(y_6 + \frac{1}{4}\right) \hat{\mathbf{x}} - \frac{1}{4}a \hat{\mathbf{y}} - c \left(z_6 - \frac{1}{4}\right) \hat{\mathbf{z}} & (16h) & S III \\
\mathbf{B}_{40} &= -z_6 \mathbf{a}_1 - \left(y_6 + z_6\right) \mathbf{a}_2 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_3 & = & -a \left(y_6 - \frac{1}{4}\right) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - c \left(z_6 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16h) & S III
\end{aligned}$$

## References

- [1] N. S. Rampersadh, A. M. Venter, and D. G. Billing, *Rietveld refinement of In<sub>2</sub>S<sub>3</sub> using neutron and X-ray powder diffraction data*, Physica B **350**, e383–e385 (2004), doi:10.1016/j.physb.2004.03.102.