

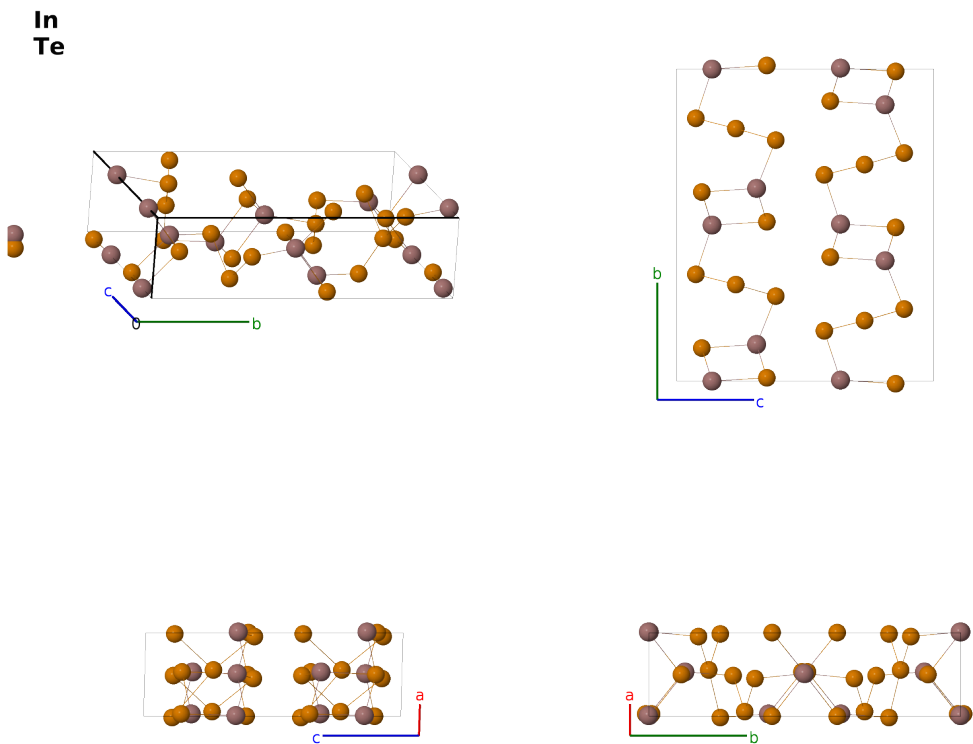
In₂Te₅ (I) Structure: A2B5_mC28_9_2a_5a-001

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<https://aflow.org/prototype-encyclopedia/FD0C>

https://aflow.org/prototype-encyclopedia/A2B5_mC28_9_2a_5a-001



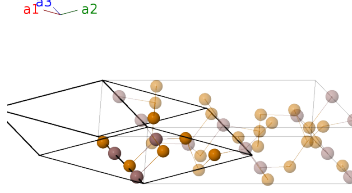
Prototype	In ₂ Te ₅
AFLOW prototype label	A2B5_mC28_9_2a_5a-001
ICSD	501
CCDC	1590994
Pearson symbol	mC28
Space group number	9
Space group symbol	<i>Cc</i>

AFLOW prototype command `aflow --proto=A2B5_mC28_9_2a_5a-001`
 `--params=a,b/a,c/a, $\beta$ , $x_1$ , $y_1$ , $z_1$ , $x_2$ , $y_2$ , $z_2$ , $x_3$ , $y_3$ , $z_3$ , $x_4$ , $y_4$ , $z_4$ , $x_5$ , $y_5$ , $z_5$ , $x_6$ , $y_6$ , $z_6$ , $x_7$ , $y_7$ , $z_7$`

- (Sutherland, 1976) found this structure, which we call In_2Te_5 (I), but later also found evidence of another tetragonal structure in the same sample. (Walton, 1978) investigated this new structure, which they called In_2Te_5 (II). (Villars, 2018) and others list In_2Te_5 (I) as the room temperature structure.
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Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$(x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4a)	In I
$\mathbf{B}_2$	$(x_1 + y_1) \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	In I
$\mathbf{B}_3$	$(x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4a)	In II
$\mathbf{B}_4$	$(x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	In II
$\mathbf{B}_5$	$(x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4a)	Te I
$\mathbf{B}_6$	$(x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Te I
$\mathbf{B}_7$	$(x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4a)	Te II
$\mathbf{B}_8$	$(x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Te II
$\mathbf{B}_9$	$(x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4a)	Te III
$\mathbf{B}_{10}$	$(x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Te III
$\mathbf{B}_{11}$	$(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4a)	Te IV
$\mathbf{B}_{12}$	$(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4a)	Te IV

$$\mathbf{B}_{13} = \begin{matrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{matrix} = (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} \quad (4a) \quad \text{Te V}$$

$$\mathbf{B}_{14} = \begin{matrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + \\ c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (4a) \quad \text{Te V}$$

References

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