

α -As₂Te₃ Structure:

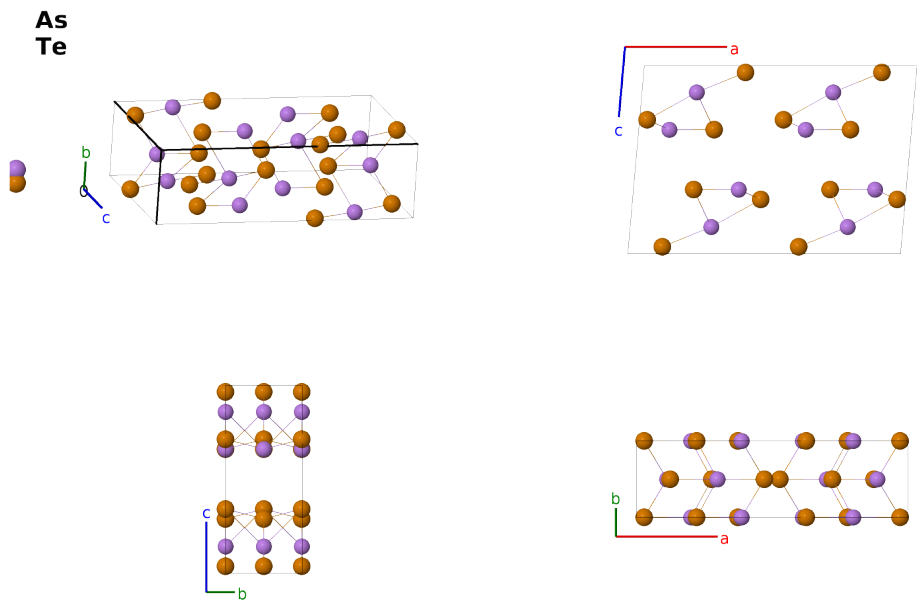
A2B3_mC20_12_2i_3i-003

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<https://aflow.org/prototype-encyclopedia/8W6Z>

https://aflow.org/prototype-encyclopedia/A2B3_mC20_12_2i_3i-003



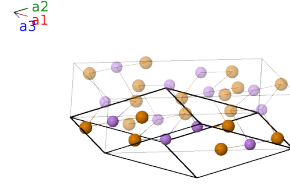
Prototype	As ₂ Te ₃
AFLOW prototype label	A2B3_mC20_12_2i_3i-003
ICSD	196146
CCDC	1704688
Pearson symbol	mC20
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A2B3_mC20_12_2i_3i-003 --params=a,b/a,c/a,β,x₁,z₁,x₂,z₂,x₃,z₃,x₄,z₄,x₅,z₅</pre>

- The ICSD entry lists Gd₂Cl₃ as the prototype, but we find that the structures are different enough to warrant giving α -As₂Te₃ its own entry.
- As₂Te₃ can also be found as β -As₂Te₃, which has the $C33$ (Bi₂Te₃) structure. (Morin, 2015)

- There are numerous structures with the AFLOW prototype label A2B3_mC20_12_2i_3i or A3B2_mC20_12_3i_2i. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- We have identified the following structures as sufficiently different to warrant their own prototypes:
 - Prototypes with the label A2B3_mC20_12_2i_3i:
 - * β -Ga₂O₃
 - * α -As₂Te₃ (this structure)
 - Prototypes with the label A3B2_mC20_12_3i_2i:
 - * Mo₂As₃
 - * Gd₂Cl₃

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
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	As I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	As I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	As II
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	As II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Te I
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Te I
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	Te II
$\mathbf{B}_8$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	Te II
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	Te III
$\mathbf{B}_{10}$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	Te III

References

- [1] C. Morin, S. Corallini, J. C., J.-B. Vaney, G. Delaizir, J.-C. Crivello, E. B. Lopes, A. Piarristeguy, J. Monnier, C. Candolfi, V. Nassif, G. J. Cuello, A. Pradel, A. P. Goncalves, B. Lenoir, and E. Alleno, *Polymorphism in Thermoelectric As₂Te₃*, Inorg. Chem. **54**, 9936–9947 (2015), doi:10.1021/acs.inorgchem.5b01676.

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