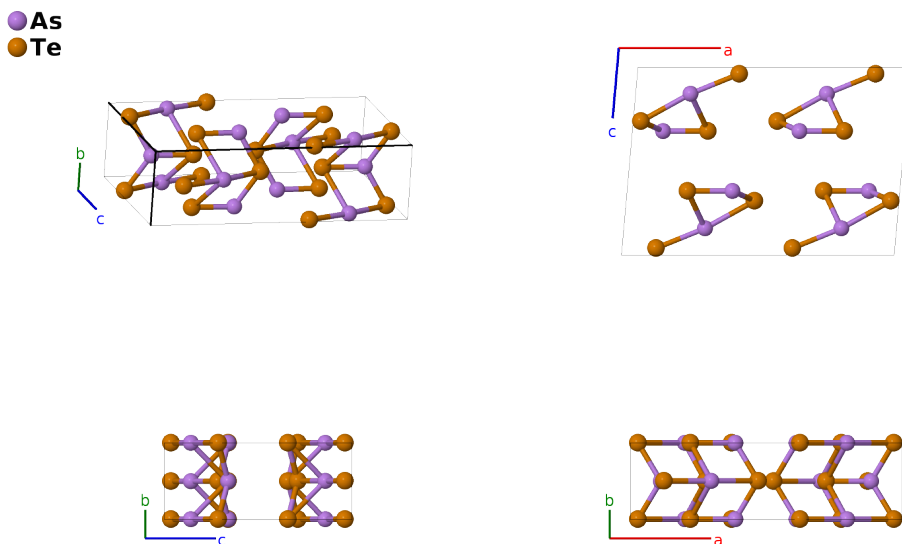


# $\alpha$ -As<sub>2</sub>Te<sub>3</sub> Structure: A2B3\_mC20\_12\_2i\_3i-003

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<https://aflow.org/p/8W6Z>

[https://aflow.org/p/A2B3\\_mC20\\_12\\_2i\\_3i-003](https://aflow.org/p/A2B3_mC20_12_2i_3i-003)



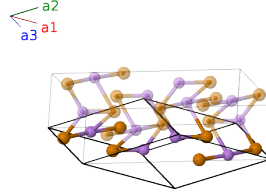
<b>Prototype</b>	As <sub>2</sub> Te <sub>3</sub>
<b>AFLOW prototype label</b>	A2B3_mC20_12_2i_3i-003
<b>ICSD</b>	196146
<b>Pearson symbol</b>	mC20
<b>Space group number</b>	12
<b>Space group symbol</b>	<i>C</i> 2/ <i>m</i>
<b>AFLOW prototype command</b>	<code>aflow --proto=A2B3_mC20_12_2i_3i-003 --params=a, b/a, c/a, <math>\beta</math>, <math>x_1</math>, <math>z_1</math>, <math>x_2</math>, <math>z_2</math>, <math>x_3</math>, <math>z_3</math>, <math>x_4</math>, <math>z_4</math>, <math>x_5</math>, <math>z_5</math></code>

- The ICSD entry lists Gd<sub>2</sub>Cl<sub>3</sub> as the prototype, but we find that the structures are different enough to warrant giving  $\alpha$ -As<sub>2</sub>Te<sub>3</sub> its own entry.
- As<sub>2</sub>Te<sub>3</sub> can also be found as  $\beta$ -As<sub>2</sub>Te<sub>3</sub>, which has the *C*33 (Bi<sub>2</sub>Te<sub>3</sub>) 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:

- \*  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>
- \*  $\alpha$ -As<sub>2</sub>Te<sub>3</sub> (this structure)
- Prototypes with the label A3B2\_mC20\_12\_3i\_2i:
  - \* Mo<sub>2</sub>As<sub>3</sub>
  - \* Gd<sub>2</sub>Cl<sub>3</sub>

### 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 As<sub>2</sub>Te<sub>3</sub>*, *Inorg. Chem.* **54**, 9936–9947 (2015), doi:10.1021/acs.inorgchem.5b01676.