

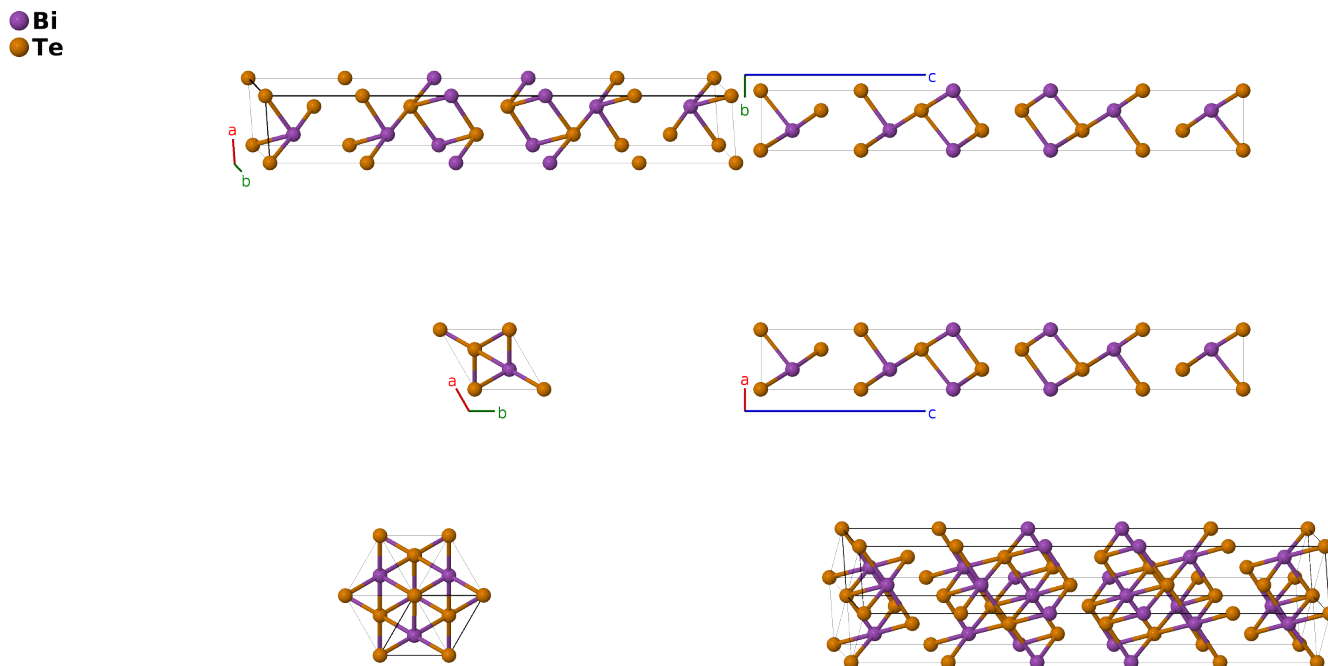
Bi₂Te₃ (C33) Structure: A2B3_hR5_166_c_ac-001

This structure originally had the label **A2B3_hR5_166_c_ac**. Calls to that address will be redirected here.

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<https://aflow.org/p/NGV5>

https://aflow.org/p/A2B3_hR5_166_c_ac-001



Prototype	Bi ₂ Te ₃
AFLOW prototype label	A2B3_hR5_166_c_ac-001
<i>Strukturbericht</i> designation	C33
ICSD	15753
Pearson symbol	hR5
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A2B3_hR5_166_c_ac-001 --params=a, c/a, x₂, x₃</code>

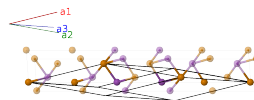
Other compounds with this structure

β -As₂Te₃, Bi₂Te₂S, Bi₂Se₃, Bi₂Te₂Se, Ga₂Te₅, In₂Te₃, Sb₂Te₃

- (Gottfried, 1937) assigns $\text{Bi}_2\text{Te}_2\text{S}$ as the prototype for *Strukturbericht* symbol *C33*, but (Lange, 1939) shows that this is isostructural with Bi_2Te_3 , the sulfur atom being replaced by a tellurium atom. We will therefore retain our original designation.
- Hexagonal settings for rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	=	0	(1a)	Te I
\mathbf{B}_2	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	=	$cx_2 \hat{\mathbf{z}}$	(2c)	Bi I
\mathbf{B}_3	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	=	$-cx_2 \hat{\mathbf{z}}$	(2c)	Bi I
\mathbf{B}_4	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$cx_3 \hat{\mathbf{z}}$	(2c)	Te II
\mathbf{B}_5	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-cx_3 \hat{\mathbf{z}}$	(2c)	Te II

References

- [1] P. W. Lange, *Ein Vergleich zwischen Bi_2Te_3 und $\text{Bi}_2\text{Te}_2\text{S}$* , *Naturwissenschaften* **27**, 133–134 (1939), doi:10.1007/BF01490284.
- [2] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).