

Bi₄Te₃ Structure:

A4B3_hR7_166_2c_ac-002

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

https://aflow.org/prototype-encyclopedia/A4B3_hR7_166_2c_ac-002

Prototype	Bi ₄ Te ₃
AFLOW prototype label	A4B3_hR7_166_2c_ac-002
ICSD	30526
CCDC	1604795
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A4B3_hR7_166_2c_ac-002</code> <code>--params=$a, c/a, x_2, x_3, x_4$</code>

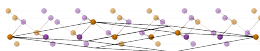
Other compounds with this structure

Bi₄Se₃

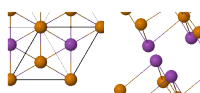
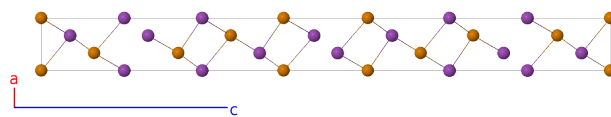
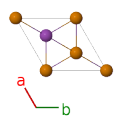
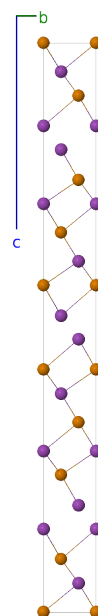
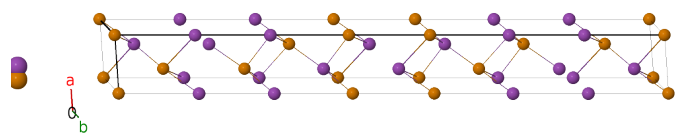
- (Villars, 2016) lists Bi₄Se₃ as the prototype for this structure, but the data for Bi₄Te₃ is much more accessible, so we use that instead.
- Al₄C₃ (*D*7₁) and Bi₄Te₃ have the same AFLOW prototype label, A4B3_hR7_166_2c_ac. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings for rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

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



Bi
Te



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) Bi 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) Bi II
$\mathbf{B}_6$	=	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	=	$cx_4 \hat{\mathbf{z}}$	(2c) Te II
$\mathbf{B}_7$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	=	$-cx_4 \hat{\mathbf{z}}$	(2c) Te II

References

- [1] K. Yamana, K. Kihara, and T. Matsumoto, *Bismuth Tellurides: BiTe and Bi₄Te₃*, Acta Crystallogr. Sect. B **35**, 147–149 (1979), doi:10.1107/S0567740879002788.
- [2] P. Villars, *Bi₄Se₃ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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