

Ti₂InB₂ Structure:

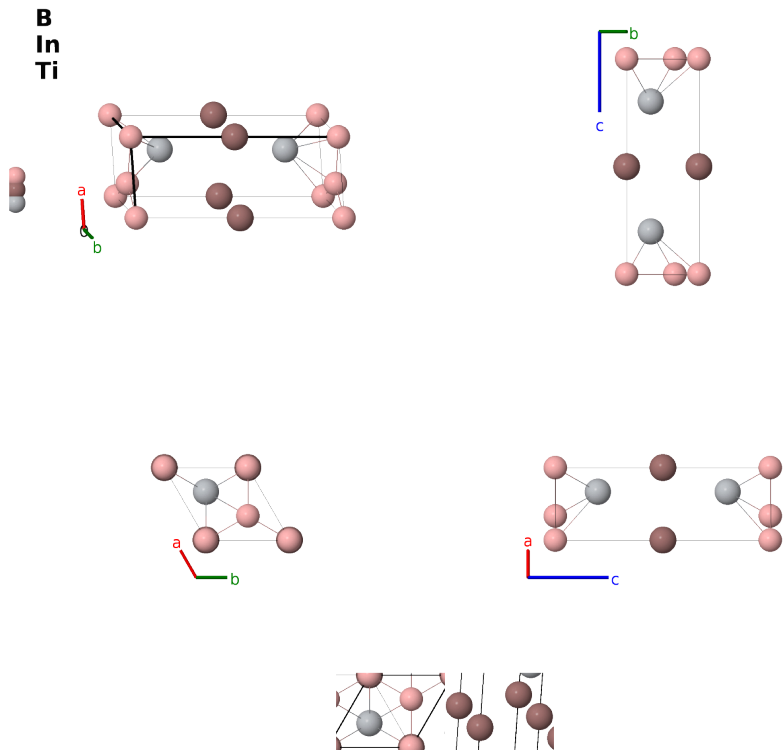
A2BC2_hP5_187_ac_b_i-001

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

https://aflow.org/prototype-encyclopedia/A2BC2_hP5_187_ac_b_i-001



Prototype	B ₂ InTi ₂
AFLOW prototype label	A2BC2_hP5_187_ac_b_i-001
Pearson symbol	hP5
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	<code>aflow --proto=A2BC2_hP5_187_ac_b_i-001</code> <code>--params=a, c/a, z₄</code>

Other compounds with this structure

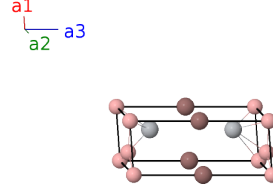
Hf₂InB₂, Hf₂SnB₂, Zr₂InB₂, Zr₂TiB₂

- (Wang, 2019) synthesized Ti₂InB₂ and found it was in space group $P\bar{6}m2$ #187, but did not give experimental positions of the atoms. Instead we use their computational results.

- We shifted the origin of the (Wang, 2019) primitive cell so that one of the boron atoms is at the origin.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(1a) B I
$\mathbf{B}_2$	$=$	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}c\hat{\mathbf{z}}$	(1b) In I
$\mathbf{B}_3$	$=$	$\frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}}$	(1c) B II
$\mathbf{B}_4$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + z_4\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(2i) Ti I
$\mathbf{B}_5$	$=$	$\frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_4\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(2i) Ti I

References

- [1] J. Wang, T.-N. Ye, Y. Gong, J. Wu, N. Miao, T. Tada, and H. Hosono, *Discovery of hexagonal ternary phase Ti_2InB_2 and its evolution to layered boride TiB* , Nat. Commun. **10**, 2284 (2019), doi:10.1038/s41467-019-10297-8.

Found in

- [1] M. A. Ali, M. M. Hossain, M. M. Uddin, A. K. M. A. Islam, and S. H. Naqib, *Understanding the improvement of thermo-mechanical and optical properties of 212 MAX phase borides Zr_2AB_2 ($A = In, Tl$)*, J. Mater. Res. Tech. **15**, 2227–2239 (2021), doi:10.1016/j.jmrt.2021.09.042.

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