Ti_2InB_2 Structure: A2BC2_hP5_187_ac_b_i-001

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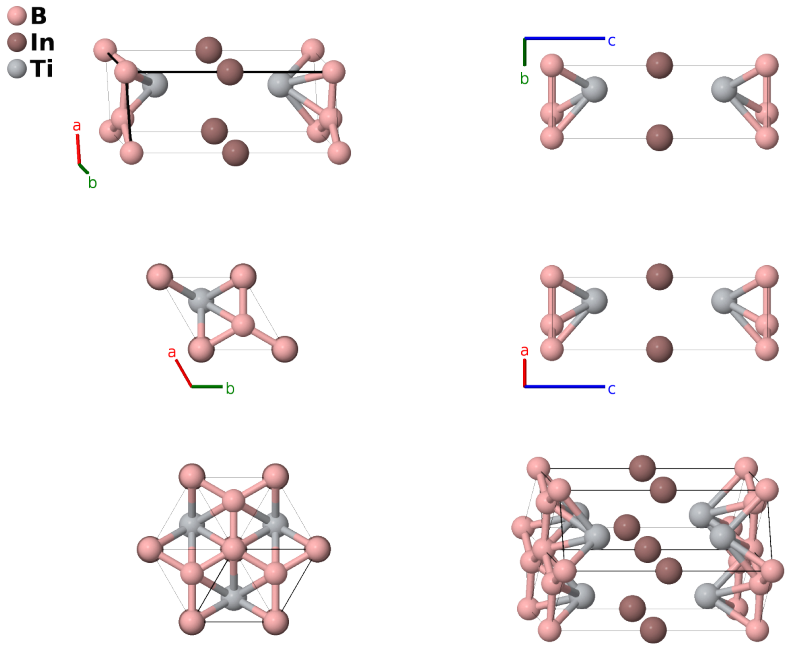
https://aflow.org/p/AJFU

https://aflow.org/p/A2BC2_hP5_187_ac_b_i-001



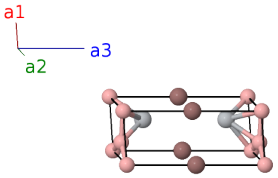
Prototype	B_2InTi_2
AFLOW prototype label	A2BC2_hP5_187_ac_b_i-001
ICSD	none
Pearson symbol	hP5
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	`aflow --proto=A2BC2_hP5_187_ac_b_i-001 --params=`$a, c/a, z_4$

Other compounds with this structure
Hf_2InB_2, Hf_2SnB_2, Zr_2InB_2, Zr_2TlB_2

- (Wang, 2019) synthesized Ti_2InB_2 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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.