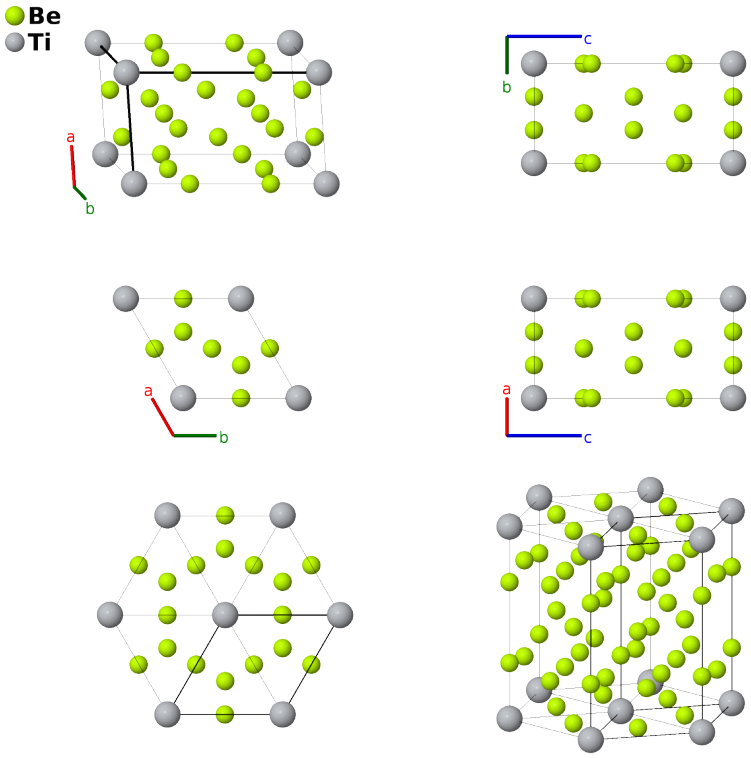
$D2_a$ ($TiBe_{12}$) Structure: A12B_hP13_191_cdei_a-001

This structure originally had the label `A12B_hP13_191_cdei_a`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/FEUM

https://aflow.org/p/A12B_hP13_191_cdei_a-001

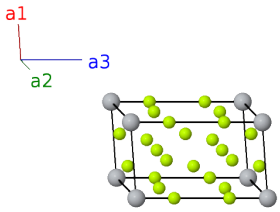


Prototype	$Be_{12}Ti$
AFLOW prototype label	A12B_hP13_191_cdei_a-001
***Strukturbericht* designation**	$D2_a$
ICSD	58745
Pearson symbol	hP13
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	`aflow --proto=A12B_hP13_191_cdei_a-001 --params=`$a, c/a, z_4, z_5$

- The structure of $TiBe_{12}$ is not settled. (Raeuchle, 1952) described the structure as a somewhat disordered supercell containing 48 atoms with lattice constants $a = 29.44$Å and $c = 7.33$Å, but they stated that a 'pseudo-cell' existed with dimensions $a = 4.23$Å and $c = 7.33$Å. This pseudo-cell is described here, and was designated *Strukturbericht* $D2_a$ by Smithells (Brandes, 1992). Rauchle and Rundle suggested that the larger primitive cell was constructed from the multiple pseudo-cells, with the titanium atom alternating between the ($1a$) and ($1b$) Wyckoff positions.
- Other experimenters have suggested that the actual structure of $TiBe_{12}$ is tetragonal. (Jackson, 2016) presents first-principles calculations which suggest that the actual structure is the tetragonal $ThMn_{12}$ ($D2_b$) type.
- $HfFe_6Ge_6$ is the ternary form of this structure.

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)	Ti I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Be I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Be I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Be II
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Be II
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2e)	Be III
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(2e)	Be III
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6i)	Be IV
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6i)	Be IV
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(6i)	Be IV
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6i)	Be IV
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6i)	Be IV
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(6i)	Be IV

References

[1] R. F. Raeuchle and R. E. Rundle, *The Structure of TiBe$_{12}$*, Acta Cryst. **5**, 85–93 (1952), doi:10.1107/S0365110X52000186.

[2] E. A. Brandes and G. B. Brook, eds., *Smithells Metals Reference Book* (Butterworth Heinemann, Oxford, Auckland, Boston, Johannesburg, Melbourne, New Delhi, 1992), seventh edn.

Found in

[1] M. L. Jackson, P. A. Burr, and R. W. Grimes, *Resolving the structure of TiBe$_{12}$*, Acta Crystallogr. Sect. B **72**, 277–280 (2016), doi:10.1107/S205252061600322X.