

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

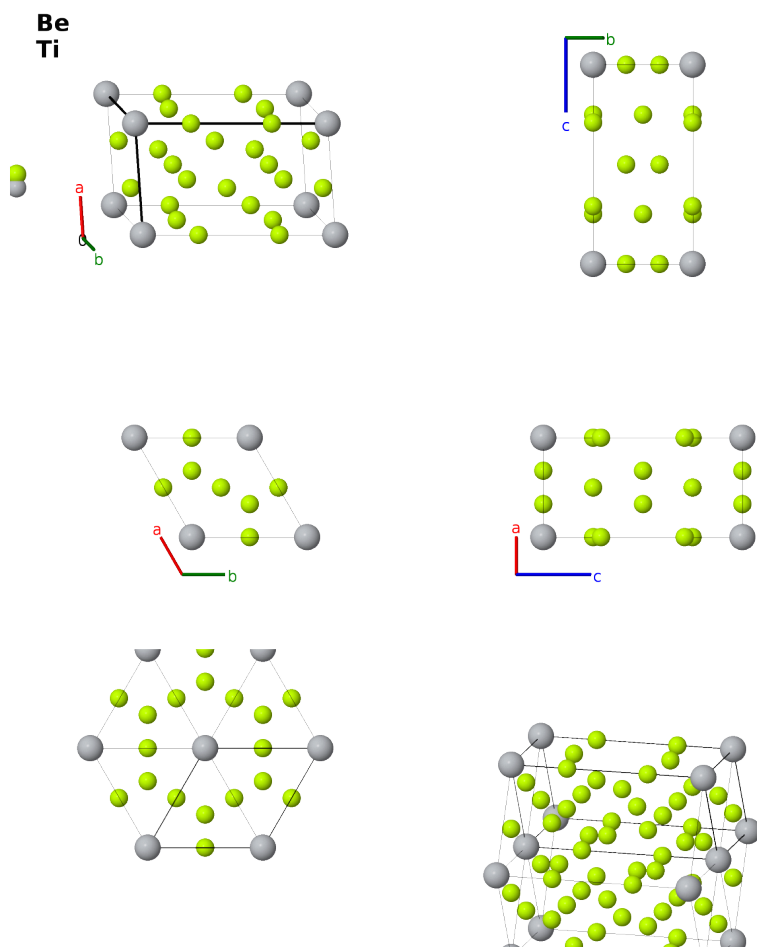
This structure previously used the label(s) **A12B_hP13_191_cdei_a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/FEUM>

https://aflow.org/prototype-encyclopedia/A12B_hP13_191_cdei_a-001



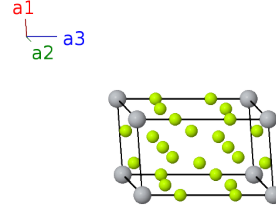
Prototype	Be_{12}Ti
AFLOW prototype label	A12B_hP13_191_cdei_a-001
<i>Strukturbericht</i> designation	$D2_a$
ICSD	58745
CCDC	1622748
Pearson symbol	hP13

Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	<code>aflow --proto=A12B_hP13_191_cdei_a-001</code> <code>--params=a, c/a, z₄, z₅</code>

- The structure of TiBe_{12} is not settled. (Raeuchle, 1952) described the structure as a somewhat disordered supercell containing 48 atoms with lattice constants $a = 29.44\text{\AA}$ and $c = 7.33\text{\AA}$, but they stated that a ‘pseudo-cell’ existed with dimensions $a = 4.23\text{\AA}$ and $c = 7.33\text{\AA}$. 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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(1a)	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.

First cited in

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.