Nb_2Be_{17} Structure: A17B2_hR19_166_cegh_c-001

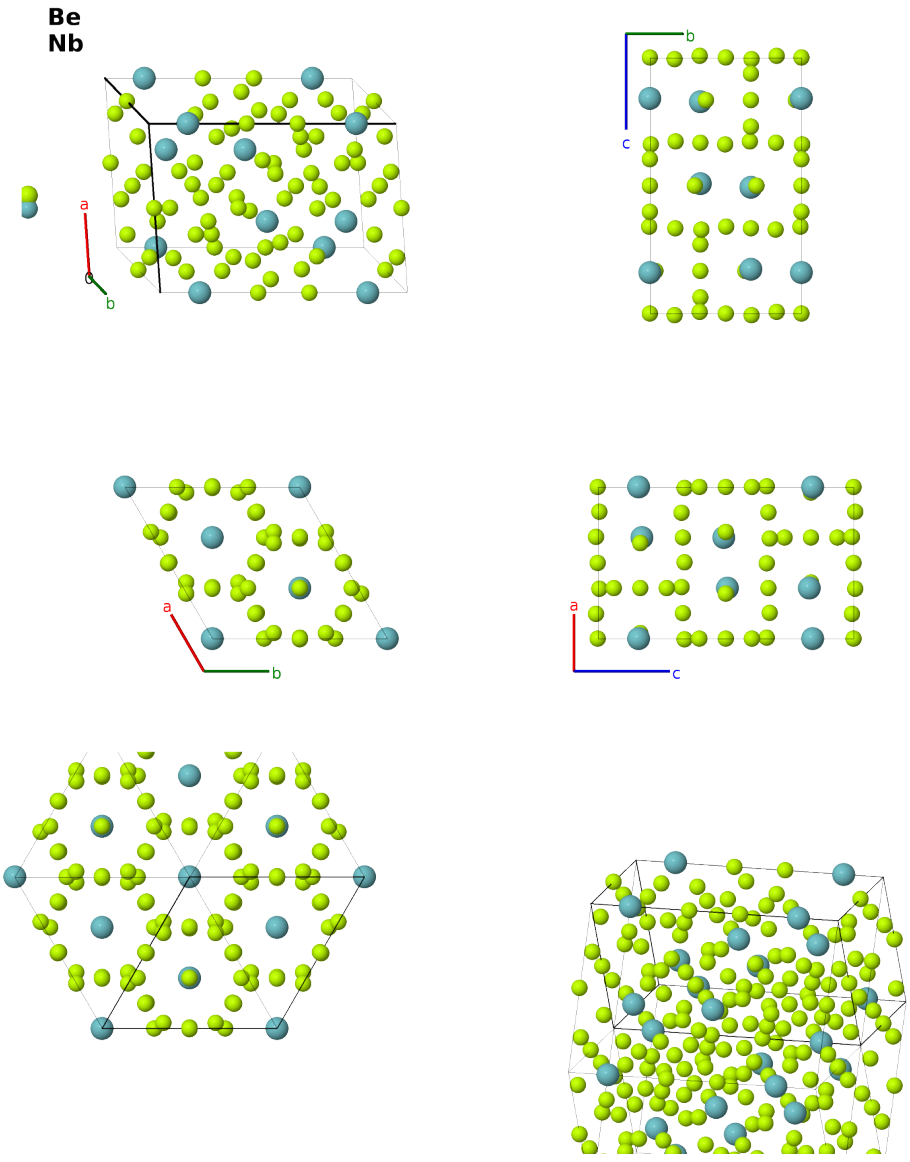
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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/3JAE

https://aflow.org/prototype-encyclopedia/A17B2_hR19_166_cegh_c-001



Prototype	$Be_{17}Nb_2$
AFLOW prototype label	A17B2_hR19_166_cegh_c-001
ICSD	58724

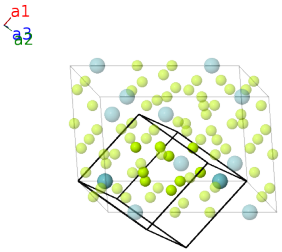
CCDC	1622727
Pearson symbol	hR19
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A17B2_hR19_166_cegh_c-001 --params=`$a, c/a, x_1, x_2, x_4, x_5, z_5$

Other compounds with this structure
α-$Be_{17}Hf_2$, $Be_{17}Ta_2$, α-$Be_{17}Ti_2$, $Be_{17}Zr_2$

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	Be I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	Be 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)	Nb I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Nb I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3e)	Be II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3e)	Be II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3e)	Be II
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2x_4 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,(6x_4 + 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	Be III
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,(2x_4 + 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,(6x_4 - 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	Be III
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	Be III
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,(2x_4 + 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{12}a\,(6x_4 - 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	Be III
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,(2x_4 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{12}a\,(6x_4 + 1)\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	Be III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6g)	Be III
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(6h)	Be IV
$\mathbf{B_{15}}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\,\hat{\mathbf{z}}$	(6h)	Be IV

$\mathbf{B_{16}}$	=	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_5 - z_5)\;\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_5 + z_5)\;\hat{\mathbf{z}}$	(6h)	Be IV
$\mathbf{B_{17}}$	=	$-z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_5 + z_5)\;\hat{\mathbf{z}}$	(6h)	Be IV
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - z_5)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - z_5)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_5 + z_5)\;\hat{\mathbf{z}}$	(6h)	Be IV
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_5 - z_5)\;\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_5 + z_5)\;\hat{\mathbf{z}}$	(6h)	Be IV

References

[1] A. Zalkin, D. E. Sands, and O. H. Krikorian, *The crystal structure of Nb_2Be_{17}*, Acta Cryst. **12**, 713–715 (1967), doi:10.1107/S0365110X59002110.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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.