

Bi₅Nb₃O₁₅ Structure:

A5B3C15_oP46_30_a2c_bc_a7c-001

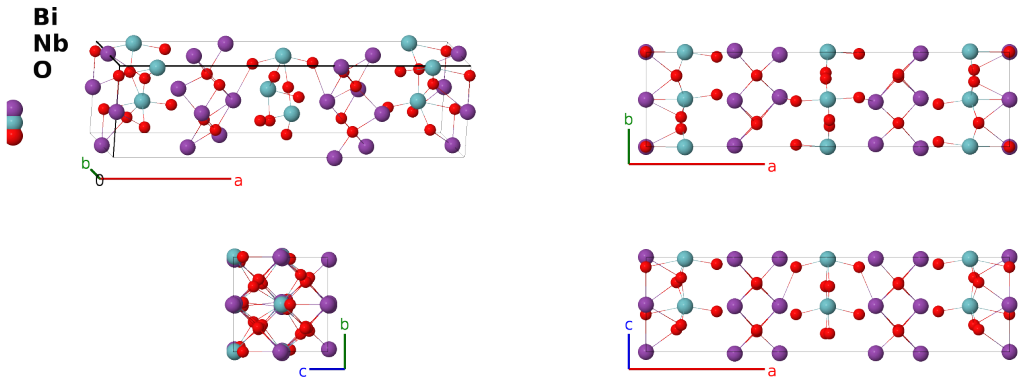
This structure previously used the label(s) **A5B3C15_oP46_30_a2c_bc_a7c**. Calls to these addresses will be redirected here.

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. Osos, 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/ABT7>

https://aflow.org/prototype-encyclopedia/A5B3C15_oP46_30_a2c_bc_a7c-001

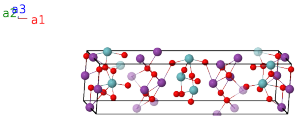


Prototype	Bi ₅ O ₁₅ Nb ₃
AFLOW prototype label	A5B3C15_oP46_30_a2c_bc_a7c-001
ICSD	245707
CCDC	1712390
Pearson symbol	oP46
Space group number	30
Space group symbol	<i>Pnc</i> 2
AFLOW prototype command	<pre>aflow --proto=A5B3C15_oP46_30_a2c_bc_a7c-001 --params=a, b/a, c/a, z₁, z₂, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁, x₁₂, y₁₂, z₁₂, x₁₃, y₁₃, z₁₃</pre>

- Our previous rendition (Hicks, 2019) of this structure had multiple errors in the CIF. We have corrected these here.
- Space group *Pnc*2 #30 allows an arbitrary choice for the origin of the *z*-axis. We fix it here by setting $z_1 = 1/2$.

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	Bi I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Bi I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c z_3 \hat{\mathbf{z}}$	(2b)	Nb I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Nb I
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} - b (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} + b (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B}_{12}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} - b (y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} + b (y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B}_{15}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B}_{16}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B}_{17}$	$= x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} - b (y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} + b (y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B}_{19}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a x_7 \hat{\mathbf{x}} + b y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{20}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a x_7 \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{21}$	$= x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_7 \hat{\mathbf{x}} - b (y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{22}$	$= -x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_7 \hat{\mathbf{x}} + b (y_7 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_{23}$	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$a x_8 \hat{\mathbf{x}} + b y_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{24}$	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a x_8 \hat{\mathbf{x}} - b y_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{25}$	$= x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_8 \hat{\mathbf{x}} - b (y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{26}$	$= -x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_8 \hat{\mathbf{x}} + b (y_8 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{27}$	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$a x_9 \hat{\mathbf{x}} + b y_9 \hat{\mathbf{y}} + c z_9 \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{28}$	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-a x_9 \hat{\mathbf{x}} - b y_9 \hat{\mathbf{y}} + c z_9 \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{29}$	$= x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_9 \hat{\mathbf{x}} - b (y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{30}$	$= -x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_9 \hat{\mathbf{x}} + b (y_9 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B}_{31}$	$= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$a x_{10} \hat{\mathbf{x}} + b y_{10} \hat{\mathbf{y}} + c z_{10} \hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B}_{32}$	$= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-a x_{10} \hat{\mathbf{x}} - b y_{10} \hat{\mathbf{y}} + c z_{10} \hat{\mathbf{z}}$	(4c)	O V

$$\begin{aligned}
\mathbf{B}_{33} &= x_{10} \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} - b \left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{O V} \\
\mathbf{B}_{34} &= -x_{10} \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} + b \left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{O V} \\
\mathbf{B}_{35} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(4c) &\quad \text{O VI} \\
\mathbf{B}_{36} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(4c) &\quad \text{O VI} \\
\mathbf{B}_{37} &= x_{11} \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 &= ax_{11} \hat{\mathbf{x}} - b \left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{O VI} \\
\mathbf{B}_{38} &= -x_{11} \mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{11} \hat{\mathbf{x}} + b \left(y_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{11} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{O VI} \\
\mathbf{B}_{39} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} &(4c) &\quad \text{O VII} \\
\mathbf{B}_{40} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= -ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} &(4c) &\quad \text{O VII} \\
\mathbf{B}_{41} &= x_{12} \mathbf{a}_1 - \left(y_{12} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 &= ax_{12} \hat{\mathbf{x}} - b \left(y_{12} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{12} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{O VII} \\
\mathbf{B}_{42} &= -x_{12} \mathbf{a}_1 + \left(y_{12} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{12} \hat{\mathbf{x}} + b \left(y_{12} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{12} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{O VII} \\
\mathbf{B}_{43} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} &(4c) &\quad \text{O VIII} \\
\mathbf{B}_{44} &= -x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= -ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} &(4c) &\quad \text{O VIII} \\
\mathbf{B}_{45} &= x_{13} \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 &= ax_{13} \hat{\mathbf{x}} - b \left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{O VIII} \\
\mathbf{B}_{46} &= -x_{13} \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{13} \hat{\mathbf{x}} + b \left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\quad \text{O VIII}
\end{aligned}$$

References

- [1] S. Tahara, A. Shimada, N. Kumada, and Y. Sugahara, *Characterization of Bi5Nb3O15 by refinement of neutron diffraction pattern, acid treatment and reaction of the acid-treated product with n-alkylamines*, J. Solid State Chem. **180**, 2517–2524 (2007), doi:10.1016/j.jssc.2007.05.017.
- [2] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

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First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043