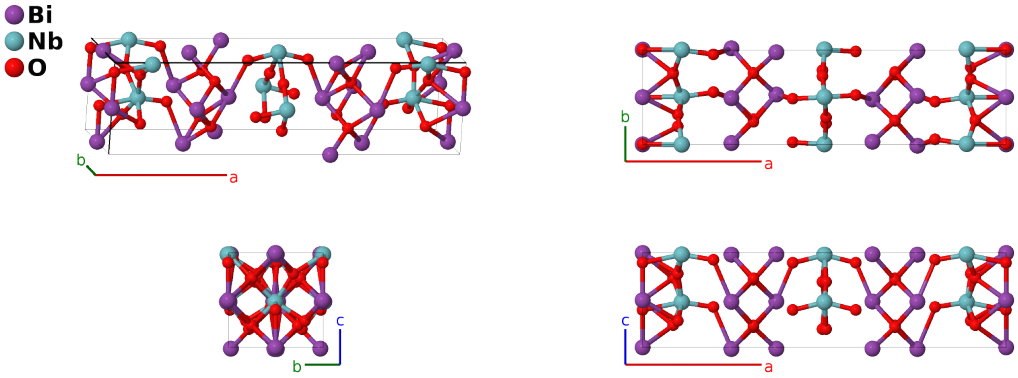
$Bi_5Nb_3O_{15}$ Structure: A5B3C15_oP46_30_a2c_bc_a7c-001

This structure originally had the label `A5B3C15_oP46_30_a2c_bc_a7c`. Calls to that address will be redirected here.

Cite this page as: 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

https://aflow.org/p/ABT7

https://aflow.org/p/A5B3C15_oP46_30_a2c_bc_a7c-001

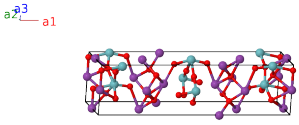


Prototype	$Bi_5O_{15}Nb_3$
AFLOW prototype label	A5B3C15_oP46_30_a2c_bc_a7c-001
ICSD	245707
Pearson symbol	oP46
Space group number	30
Space group symbol	$Pnc2$
AFLOW prototype command	`aflow --proto=A5B3C15_oP46_30_a2c_bc_a7c-001 --params=`$a, b/a, c/a, z_1, z_2, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}$

- Our previous rendition (Hicks, 2019) of this structure had multiple errors in the CIF. We have corrected these here.
- Space group $Pnc2$ #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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Bi I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Bi I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(2b)	Nb I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Nb I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Bi II
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Bi III
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B_{16}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Nb II
$\mathbf{B_{19}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{20}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{21}}$	=	$x_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{22}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{23}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{24}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{25}}$	=	$x_8\,\mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{26}}$	=	$-x_8\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{27}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B_{28}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B_{29}}$	=	$x_9\,\mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B_{30}}$	=	$-x_9\,\mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O IV
$\mathbf{B_{31}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B_{32}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4c)	O V
$\mathbf{B_{33}}$	=	$x_{10}\,\mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} - b\left(y_{10} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	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)	O VIII

References

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[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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