β-NbO_2 Structure: AB2_tI48_80_2b_4b-001

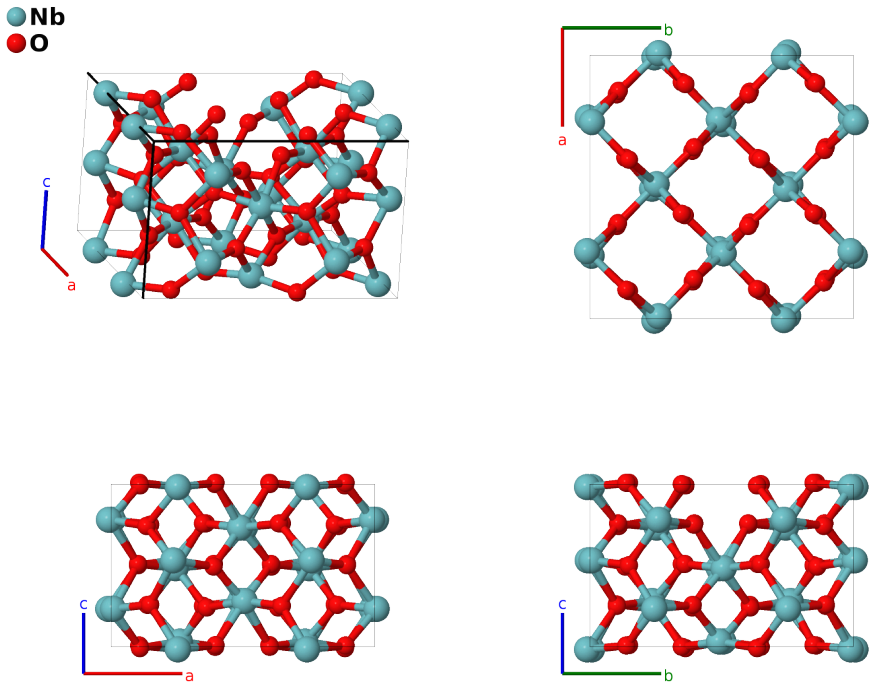
This structure originally had the label `AB2_tI48_80_2b_4b`. Calls to that address will be redirected here.

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/2XGR

https://aflow.org/p/AB2_tI48_80_2b_4b-001

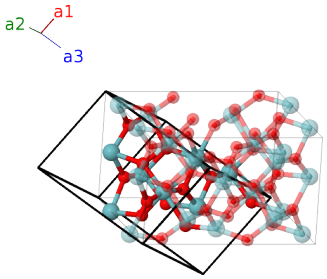


Prototype	NbO_2
AFLOW prototype label	AB2_tI48_80_2b_4b-001
ICSD	35181
Pearson symbol	tI48
Space group number	80
Space group symbol	$I4_1$
AFLOW prototype command	`aflow --proto=AB2_tI48_80_2b_4b-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- The actual composition is $Nb_{2-x}O_2$, with $0.002 < x < 0.1$.
- NbO_2 can also be found in the α-NbO_2 structure.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(y_1+z_1)\,\mathbf{a}_1+(x_1+z_1)\,\mathbf{a}_2+(x_1+y_1)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}+ay_1\,\hat{\mathbf{y}}+cz_1\,\hat{\mathbf{z}}$	(8b)	Nb I
$\mathbf{B_2}$	=	$-(y_1-z_1)\,\mathbf{a}_1-(x_1-z_1)\,\mathbf{a}_2-(x_1+y_1)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}-ay_1\,\hat{\mathbf{y}}+cz_1\,\hat{\mathbf{z}}$	(8b)	Nb I
$\mathbf{B_3}$	=	$\left(x_1+z_1+\frac{3}{4}\right)\,\mathbf{a}_1+\left(-y_1+z_1+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_1-y_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_1\,\hat{\mathbf{x}}+a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_1+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Nb I
$\mathbf{B_4}$	=	$\left(-x_1+z_1+\frac{3}{4}\right)\,\mathbf{a}_1+\left(y_1+z_1+\frac{1}{4}\right)\,\mathbf{a}_2+\left(-x_1+y_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_1\,\hat{\mathbf{x}}-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_1+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Nb I
$\mathbf{B_5}$	=	$(y_2+z_2)\,\mathbf{a}_1+(x_2+z_2)\,\mathbf{a}_2+(x_2+y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}+ay_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8b)	Nb II
$\mathbf{B_6}$	=	$-(y_2-z_2)\,\mathbf{a}_1-(x_2-z_2)\,\mathbf{a}_2-(x_2+y_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}-ay_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(8b)	Nb II
$\mathbf{B_7}$	=	$\left(x_2+z_2+\frac{3}{4}\right)\,\mathbf{a}_1+\left(-y_2+z_2+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_2-y_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}}+a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Nb II
$\mathbf{B_8}$	=	$\left(-x_2+z_2+\frac{3}{4}\right)\,\mathbf{a}_1+\left(y_2+z_2+\frac{1}{4}\right)\,\mathbf{a}_2+\left(-x_2+y_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}}-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	Nb II
$\mathbf{B_9}$	=	$(y_3+z_3)\,\mathbf{a}_1+(x_3+z_3)\,\mathbf{a}_2+(x_3+y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{10}}$	=	$-(y_3-z_3)\,\mathbf{a}_1-(x_3-z_3)\,\mathbf{a}_2-(x_3+y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{11}}$	=	$\left(x_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_1+\left(-y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_2+\left(x_3-y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}}+a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{12}}$	=	$\left(-x_3+z_3+\frac{3}{4}\right)\,\mathbf{a}_1+\left(y_3+z_3+\frac{1}{4}\right)\,\mathbf{a}_2+\left(-x_3+y_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}}-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{13}}$	=	$(y_4+z_4)\,\mathbf{a}_1+(x_4+z_4)\,\mathbf{a}_2+(x_4+y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(8b)	O II

$$\mathbf{B_{14}} = -(y_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} \quad (8b) \quad \text{O II}$$

$$\mathbf{B_{15}} = \left(x_4 + z_4 + \tfrac{3}{4}\right)\mathbf{a}_1 + \left(-y_4 + z_4 + \tfrac{1}{4}\right)\mathbf{a}_2 + \left(x_4 - y_4 + \tfrac{1}{2}\right)\mathbf{a}_3 = -ay_4\,\hat{\mathbf{x}} + a\left(x_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O II}$$

$$\mathbf{B_{16}} = \left(-x_4 + z_4 + \tfrac{3}{4}\right)\mathbf{a}_1 + \left(y_4 + z_4 + \tfrac{1}{4}\right)\mathbf{a}_2 + \left(-x_4 + y_4 + \tfrac{1}{2}\right)\mathbf{a}_3 = ay_4\,\hat{\mathbf{x}} - a\left(x_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O II}$$

$$\mathbf{B_{17}} = (y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad (8b) \quad \text{O III}$$

$$\mathbf{B_{18}} = -(y_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad (8b) \quad \text{O III}$$

$$\mathbf{B_{19}} = \left(x_5 + z_5 + \tfrac{3}{4}\right)\mathbf{a}_1 + \left(-y_5 + z_5 + \tfrac{1}{4}\right)\mathbf{a}_2 + \left(x_5 - y_5 + \tfrac{1}{2}\right)\mathbf{a}_3 = -ay_5\,\hat{\mathbf{x}} + a\left(x_5 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O III}$$

$$\mathbf{B_{20}} = \left(-x_5 + z_5 + \tfrac{3}{4}\right)\mathbf{a}_1 + \left(y_5 + z_5 + \tfrac{1}{4}\right)\mathbf{a}_2 + \left(-x_5 + y_5 + \tfrac{1}{2}\right)\mathbf{a}_3 = ay_5\,\hat{\mathbf{x}} - a\left(x_5 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O III}$$

$$\mathbf{B_{21}} = (y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (8b) \quad \text{O IV}$$

$$\mathbf{B_{22}} = -(y_6 - z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (8b) \quad \text{O IV}$$

$$\mathbf{B_{23}} = \left(x_6 + z_6 + \tfrac{3}{4}\right)\mathbf{a}_1 + \left(-y_6 + z_6 + \tfrac{1}{4}\right)\mathbf{a}_2 + \left(x_6 - y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = -ay_6\,\hat{\mathbf{x}} + a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O IV}$$

$$\mathbf{B_{24}} = \left(-x_6 + z_6 + \tfrac{3}{4}\right)\mathbf{a}_1 + \left(y_6 + z_6 + \tfrac{1}{4}\right)\mathbf{a}_2 + \left(-x_6 + y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = ay_6\,\hat{\mathbf{x}} - a\left(x_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (8b) \quad \text{O IV}$$

References

[1] H.-J. Schweizer and R. Gruehn, *Zur Darstellung und Kristallstruktur von β-NbO_2*, Z. f. Naturf. B **37**, 1361–1368 (1982), doi:10.1515/znb-1982-1101.

Found in

[1] P. Villars and L. D. Calvert, eds., *Pearson's Handbook of Crystallographic Data* (ASM International, Materials Park OH, 1991), vol. IV, chap. , p. 4535.