

# $\beta$ -NbO<sub>2</sub> Structure:

## AB2\_tI48\_80\_2b\_4b-001

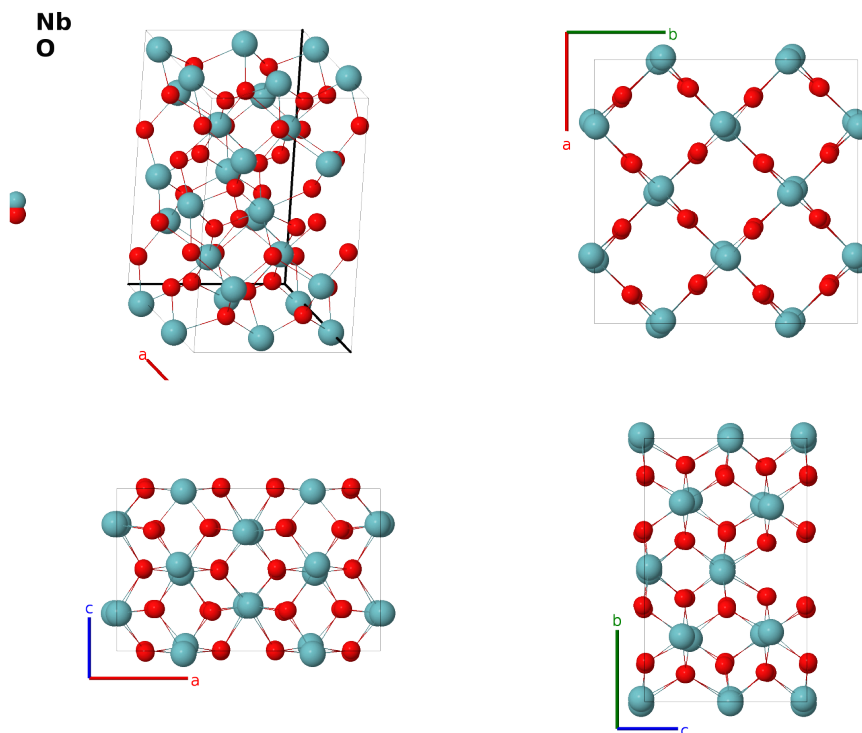
This structure previously used the label(s) **AB2\_tI48\_80\_2b\_4b**. Calls to these addresses will be redirected here.

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- 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/2XGR>

[https://aflow.org/prototype-encyclopedia/AB2\\_tI48\\_80\\_2b\\_4b-001](https://aflow.org/prototype-encyclopedia/AB2_tI48_80_2b_4b-001)



|                         |                                                                                                                                                                                                                                                                                                                                              |
|-------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype               | NbO <sub>2</sub>                                                                                                                                                                                                                                                                                                                             |
| AFLOW prototype label   | AB2_tI48_80_2b_4b-001                                                                                                                                                                                                                                                                                                                        |
| ICSD                    | 35181                                                                                                                                                                                                                                                                                                                                        |
| CCDC                    | 1607330                                                                                                                                                                                                                                                                                                                                      |
| Pearson symbol          | tI48                                                                                                                                                                                                                                                                                                                                         |
| Space group number      | 80                                                                                                                                                                                                                                                                                                                                           |
| Space group symbol      | $I4_1$                                                                                                                                                                                                                                                                                                                                       |
| AFLOW prototype command | <pre>aflow --proto=AB2_tI48_80_2b_4b-001 --params=a, c/a, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub></pre> |

- The actual composition is  $\text{Nb}_{2-x}\text{O}_2$ , with  $0.002 < x < 0.1$ .
- $\text{NbO}_2$  can also be found in the  $\alpha\text{-NbO}_2$  structure.

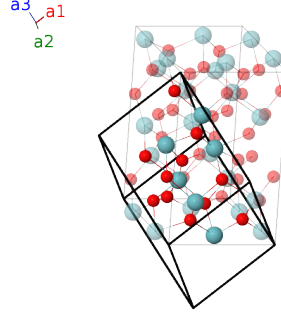
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### Body-centered Tetragonal primitive vectors

$$\mathbf{a}_1 = -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}$$




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### 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      |
| $\mathbf{B}_3$    | $= \begin{pmatrix} x_1 + z_1 + \frac{3}{4} \\ -y_1 + z_1 + \frac{1}{4} \\ x_1 - y_1 + \frac{1}{2} \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}$  | $=$ | $-ay_1 \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{4}\right) \hat{\mathbf{z}}$ | (8b)             | Nb I      |
| $\mathbf{B}_4$    | $= \begin{pmatrix} -x_1 + z_1 + \frac{3}{4} \\ y_1 + z_1 + \frac{1}{4} \\ -x_1 + y_1 + \frac{1}{2} \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}$ | $=$ | $ay_1 \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{4}\right) \hat{\mathbf{z}}$  | (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     |
| $\mathbf{B}_7$    | $= \begin{pmatrix} x_2 + z_2 + \frac{3}{4} \\ -y_2 + z_2 + \frac{1}{4} \\ x_2 - y_2 + \frac{1}{2} \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}$  | $=$ | $-ay_2 \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$ | (8b)             | Nb II     |
| $\mathbf{B}_8$    | $= \begin{pmatrix} -x_2 + z_2 + \frac{3}{4} \\ y_2 + z_2 + \frac{1}{4} \\ -x_2 + y_2 + \frac{1}{2} \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}$ | $=$ | $ay_2 \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$  | (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       |
| $\mathbf{B}_{11}$ | $= \begin{pmatrix} x_3 + z_3 + \frac{3}{4} \\ -y_3 + z_3 + \frac{1}{4} \\ x_3 - y_3 + \frac{1}{2} \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}$  | $=$ | $-ay_3 \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}}$ | (8b)             | O I       |
| $\mathbf{B}_{12}$ | $= \begin{pmatrix} -x_3 + z_3 + \frac{3}{4} \\ y_3 + z_3 + \frac{1}{4} \\ -x_3 + y_3 + \frac{1}{2} \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix}$ | $=$ | $ay_3 \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}}$  | (8b)             | O I       |

$$\begin{aligned}
\mathbf{B}_{13} &= \begin{pmatrix} (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + \\ (x_4 + y_4) \mathbf{a}_3 \end{pmatrix} = ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (8b) & \text{O II} \\
\mathbf{B}_{14} &= -\begin{pmatrix} (y_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - \\ (x_4 + y_4) \mathbf{a}_3 \end{pmatrix} = -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (8b) & \text{O II} \\
\mathbf{B}_{15} &= \begin{pmatrix} (x_4 + z_4 + \frac{3}{4}) \mathbf{a}_1 + \\ (-y_4 + z_4 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (8b) & \text{O II} \\
\mathbf{B}_{16} &= \begin{pmatrix} (-x_4 + z_4 + \frac{3}{4}) \mathbf{a}_1 + \\ (y_4 + z_4 + \frac{1}{4}) \mathbf{a}_2 + \\ (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ay_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (8b) & \text{O II} \\
\mathbf{B}_{17} &= \begin{pmatrix} (y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + \\ (x_5 + y_5) \mathbf{a}_3 \end{pmatrix} = ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (8b) & \text{O III} \\
\mathbf{B}_{18} &= -\begin{pmatrix} (y_5 - z_5) \mathbf{a}_1 - (x_5 - z_5) \mathbf{a}_2 - \\ (x_5 + y_5) \mathbf{a}_3 \end{pmatrix} = -ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (8b) & \text{O III} \\
\mathbf{B}_{19} &= \begin{pmatrix} (x_5 + z_5 + \frac{3}{4}) \mathbf{a}_1 + \\ (-y_5 + z_5 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (8b) & \text{O III} \\
\mathbf{B}_{20} &= \begin{pmatrix} (-x_5 + z_5 + \frac{3}{4}) \mathbf{a}_1 + \\ (y_5 + z_5 + \frac{1}{4}) \mathbf{a}_2 + \\ (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ay_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (8b) & \text{O III} \\
\mathbf{B}_{21} &= \begin{pmatrix} (y_6 + z_6) \mathbf{a}_1 + (x_6 + z_6) \mathbf{a}_2 + \\ (x_6 + y_6) \mathbf{a}_3 \end{pmatrix} = ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8b) & \text{O IV} \\
\mathbf{B}_{22} &= -\begin{pmatrix} (y_6 - z_6) \mathbf{a}_1 - (x_6 - z_6) \mathbf{a}_2 - \\ (x_6 + y_6) \mathbf{a}_3 \end{pmatrix} = -ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8b) & \text{O IV} \\
\mathbf{B}_{23} &= \begin{pmatrix} (x_6 + z_6 + \frac{3}{4}) \mathbf{a}_1 + \\ (-y_6 + z_6 + \frac{1}{4}) \mathbf{a}_2 + \\ (x_6 - y_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_6 \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}} & (8b) & \text{O IV} \\
\mathbf{B}_{24} &= \begin{pmatrix} (-x_6 + z_6 + \frac{3}{4}) \mathbf{a}_1 + \\ (y_6 + z_6 + \frac{1}{4}) \mathbf{a}_2 + \\ (-x_6 + y_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ay_6 \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}} & (8b) & \text{O IV}
\end{aligned}$$

## References

- [1] H.-J. Schweizer and R. Gruehn, *Zur Darstellung und Kristallstruktur von  $\beta\text{-NbO}_2$* , 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.

## 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