

α -NbO₂ Structure:

AB2_tI96_88_2f_4f-001

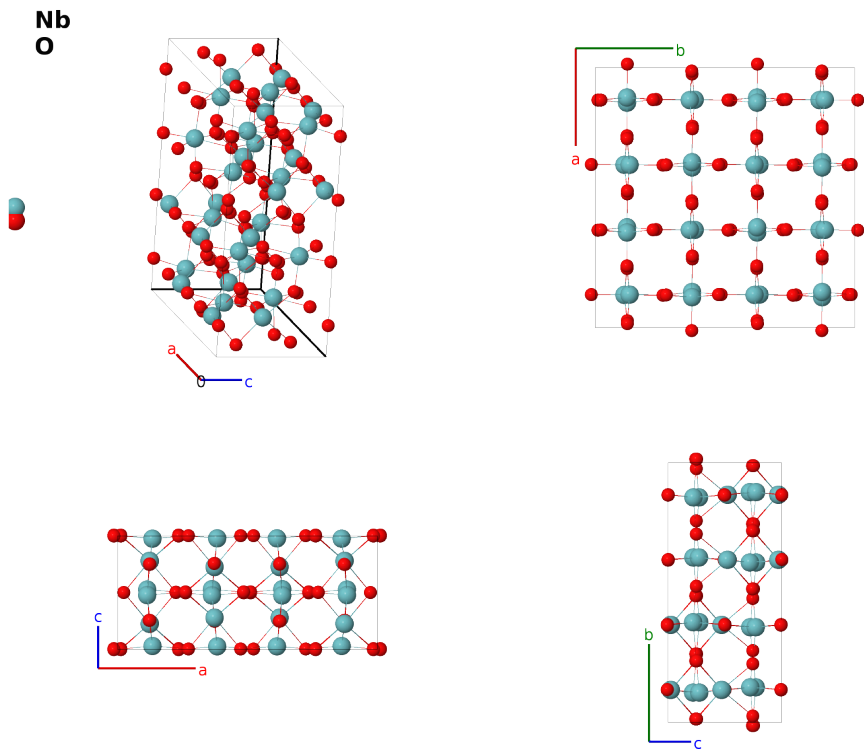
This structure previously used the label(s) **AB2_tI96_88_2f_4f**. Calls to these addresses will be redirected here.

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. 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/BLKR>

https://aflow.org/prototype-encyclopedia/AB2_tI96_88_2f_4f-001

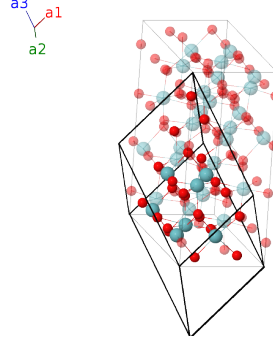


Prototype	NbO ₂
AFLOW prototype label	AB2_tI96_88_2f_4f-001
ICSD	75197
CCDC	1635861
Pearson symbol	tI96
Space group number	88
Space group symbol	$I4_1/a$
AFLOW prototype command	<pre>aflow --proto=AB2_tI96_88_2f_4f-001 --params=a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆</pre>

- NbO₂ can also be found in the β -NbO₂ structure.
- Although (Bolzan, 1994) also give structural information for α -NbO₂, (Pynn, 1996) is the only reference we found which unambiguously states that this structure is reported in setting 2 of space group $I4_1/a$ #88.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$(y_1 + z_1) \mathbf{a}_1 + (x_1 + z_1) \mathbf{a}_2 + (x_1 + y_1) \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(16f)	Nb I
$\mathbf{B}_2$	$(-y_1 + z_1 + \frac{1}{2}) \mathbf{a}_1 - (x_1 - z_1) \mathbf{a}_2 - (x_1 + y_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} - a(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(16f)	Nb I
$\mathbf{B}_3$	$(x_1 + z_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - z_1) \mathbf{a}_2 + (x_1 - y_1) \mathbf{a}_3$	=	$-a(y_1 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Nb I
$\mathbf{B}_4$	$(-x_1 + z_1 + \frac{1}{2}) \mathbf{a}_1 + (y_1 + z_1 + \frac{1}{2}) \mathbf{a}_2 + (-x_1 + y_1 + \frac{1}{2}) \mathbf{a}_3$	=	$a(y_1 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Nb I
$\mathbf{B}_5$	$-(y_1 + z_1) \mathbf{a}_1 - (x_1 + z_1) \mathbf{a}_2 - (x_1 + y_1) \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(16f)	Nb I
$\mathbf{B}_6$	$(y_1 - z_1 + \frac{1}{2}) \mathbf{a}_1 + (x_1 - z_1) \mathbf{a}_2 + (x_1 + y_1 + \frac{1}{2}) \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + a(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(16f)	Nb I
$\mathbf{B}_7$	$-(x_1 + z_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 - z_1) \mathbf{a}_2 - (x_1 - y_1) \mathbf{a}_3$	=	$a(y_1 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Nb I
$\mathbf{B}_8$	$(x_1 - z_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 + z_1 - \frac{1}{2}) \mathbf{a}_2 + (x_1 - y_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(y_1 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Nb I
$\mathbf{B}_9$	$(y_2 + z_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(16f)	Nb II
$\mathbf{B}_{10}$	$(-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - z_2) \mathbf{a}_2 - (x_2 + y_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(16f)	Nb II
$\mathbf{B}_{11}$	$(x_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - z_2) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3$	=	$-a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Nb II
$\mathbf{B}_{12}$	$(-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 + (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3$	=	$a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Nb II

$$\begin{aligned}
\mathbf{B}_{13} &= \begin{matrix} -(y_2 + z_2) \mathbf{a}_1 - (x_2 + z_2) \mathbf{a}_2 - \\ (x_2 + y_2) \mathbf{a}_3 \end{matrix} = -ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}} & (16f) & \text{Nb II} \\
\mathbf{B}_{14} &= \begin{matrix} (y_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_2 - z_2) \mathbf{a}_2 + (x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_2 \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}} & (16f) & \text{Nb II} \\
\mathbf{B}_{15} &= \begin{matrix} -(x_2 + z_2 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_2 - z_2) \mathbf{a}_2 - (x_2 - y_2) \mathbf{a}_3 \end{matrix} = a(y_2 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{Nb II} \\
\mathbf{B}_{16} &= \begin{matrix} (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_2 - y_2 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_2 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{Nb II} \\
\mathbf{B}_{17} &= \begin{matrix} (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + \\ (x_3 + y_3) \mathbf{a}_3 \end{matrix} = ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{18} &= \begin{matrix} (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{19} &= \begin{matrix} (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 - z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3 \end{matrix} = -a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{20} &= \begin{matrix} (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{21} &= \begin{matrix} -(y_3 + z_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2 - \\ (x_3 + y_3) \mathbf{a}_3 \end{matrix} = -ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{22} &= \begin{matrix} (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - z_3) \mathbf{a}_2 + (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{23} &= \begin{matrix} -(x_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 - z_3) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3 \end{matrix} = a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{24} &= \begin{matrix} (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{25} &= \begin{matrix} (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + \\ (x_4 + y_4) \mathbf{a}_3 \end{matrix} = ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{26} &= \begin{matrix} (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{27} &= \begin{matrix} (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 \end{matrix} = -a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{28} &= \begin{matrix} (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{29} &= \begin{matrix} -(y_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - \\ (x_4 + y_4) \mathbf{a}_3 \end{matrix} = -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{30} &= \begin{matrix} (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - z_4) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{31} &= \begin{matrix} -(x_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_4 - z_4) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 \end{matrix} = a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{32} &= \begin{matrix} (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O II} \\
\mathbf{B}_{33} &= \begin{matrix} (y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + \\ (x_5 + y_5) \mathbf{a}_3 \end{matrix} = ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16f) & \text{O III}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{34} &= \begin{pmatrix} -y_5 + z_5 + \frac{1}{2} \\ x_5 - z_5 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_5 + y_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -ax_5 \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} &(16f) &\text{O III} \\
\mathbf{B}_{35} &= \begin{pmatrix} x_5 + z_5 + \frac{1}{2} \\ y_5 - z_5 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_5 + y_5 \end{pmatrix} \mathbf{a}_3 &= -a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} &(16f) &\text{O III} \\
\mathbf{B}_{36} &= \begin{pmatrix} -x_5 + z_5 + \frac{1}{2} \\ y_5 + z_5 + \frac{1}{2} \\ -x_5 + y_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 &= a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} &(16f) &\text{O III} \\
\mathbf{B}_{37} &= \begin{pmatrix} -(y_5 + z_5) \\ (x_5 + y_5) \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_5 + z_5 \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 &= -ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(16f) &\text{O III} \\
\mathbf{B}_{38} &= \begin{pmatrix} y_5 - z_5 + \frac{1}{2} \\ x_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_5 + y_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= ax_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(16f) &\text{O III} \\
\mathbf{B}_{39} &= \begin{pmatrix} -(x_5 + z_5 - \frac{1}{2}) \\ y_5 - z_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_5 - y_5 \end{pmatrix} \mathbf{a}_3 &= a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} &(16f) &\text{O III} \\
\mathbf{B}_{40} &= \begin{pmatrix} x_5 - z_5 + \frac{1}{2} \\ y_5 + z_5 - \frac{1}{2} \\ x_5 - y_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \mathbf{a}_2 + \mathbf{a}_3 &= -a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} &(16f) &\text{O III} \\
\mathbf{B}_{41} &= \begin{pmatrix} y_6 + z_6 \\ x_6 + y_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_6 + z_6 \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(16f) &\text{O IV} \\
\mathbf{B}_{42} &= \begin{pmatrix} -y_6 + z_6 + \frac{1}{2} \\ x_6 - z_6 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_6 + y_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} &(16f) &\text{O IV} \\
\mathbf{B}_{43} &= \begin{pmatrix} x_6 + z_6 + \frac{1}{2} \\ y_6 - z_6 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_6 - y_6 \end{pmatrix} \mathbf{a}_3 &= -a(y_6 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}} &(16f) &\text{O IV} \\
\mathbf{B}_{44} &= \begin{pmatrix} -x_6 + z_6 + \frac{1}{2} \\ y_6 + z_6 + \frac{1}{2} \\ -x_6 + y_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 &= a(y_6 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{4}) \hat{\mathbf{z}} &(16f) &\text{O IV} \\
\mathbf{B}_{45} &= \begin{pmatrix} -(y_6 + z_6) \\ x_6 + y_6 \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_6 + z_6 \end{pmatrix} \mathbf{a}_2 - \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(16f) &\text{O IV} \\
\mathbf{B}_{46} &= \begin{pmatrix} y_6 - z_6 + \frac{1}{2} \\ x_6 - z_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_6 + y_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} &(16f) &\text{O IV} \\
\mathbf{B}_{47} &= \begin{pmatrix} -(x_6 + z_6 - \frac{1}{2}) \\ y_6 - z_6 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_6 - y_6 \end{pmatrix} \mathbf{a}_3 &= a(y_6 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{4}) \hat{\mathbf{z}} &(16f) &\text{O IV} \\
\mathbf{B}_{48} &= \begin{pmatrix} x_6 - z_6 + \frac{1}{2} \\ y_6 + z_6 - \frac{1}{2} \\ x_6 - y_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \mathbf{a}_2 + \mathbf{a}_3 &= -a(y_6 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{4}) \hat{\mathbf{z}} &(16f) &\text{O IV}
\end{aligned}$$

References

- [1] R. Pynn, J. D. Axe, and R. Thomas, *Structural distortions in the low-temperature phase of NbO₂*, Phys. Rev. B **13**, 2965–2975 (1996), doi:10.1103/PhysRevB.13.2965.

Found in

- [1] A. A. Bolzan, C. Fong, B. J. Kennedy, and C. J. Howard, *A Powder Neutron Diffraction Study of Semiconducting and Metallic Niobium Dioxide*, J. Solid State Chem. **113**, 9–14 (1994), doi:10.1006/jssc.1994.1334.

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