

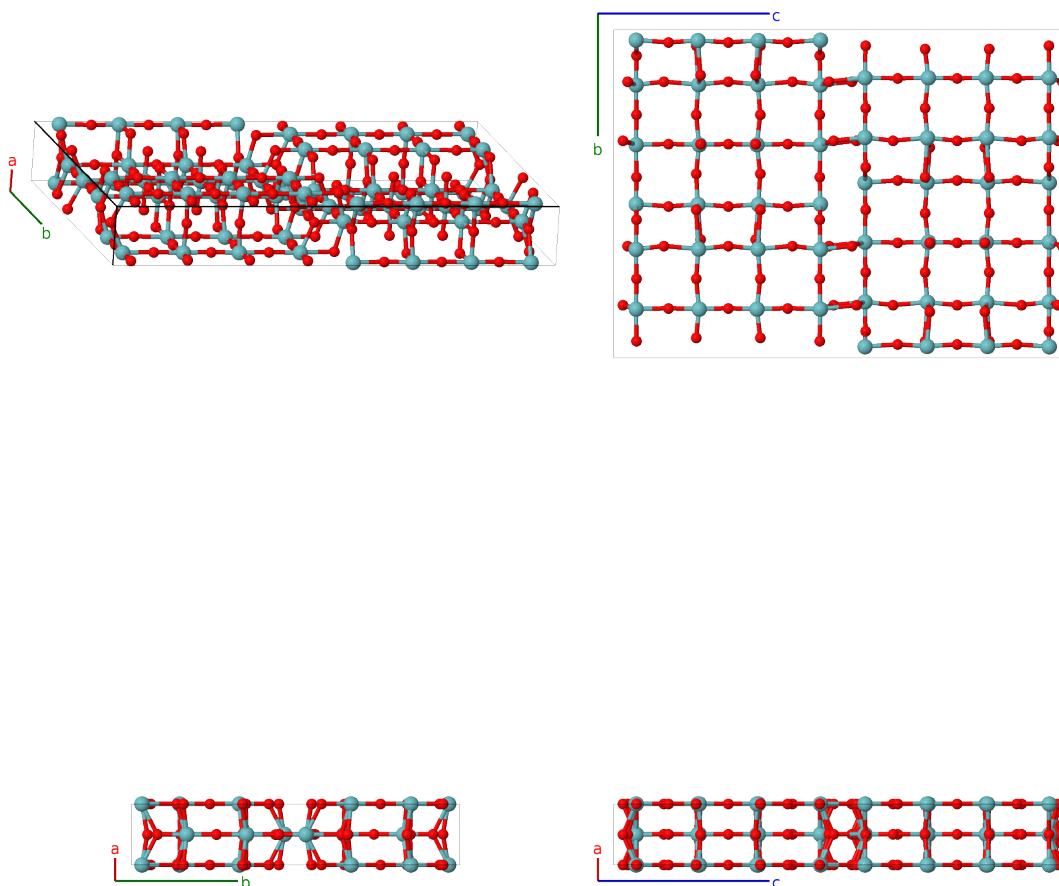
Orthorhombic Nb₁₂O₂₉ Structure: A12B29_oC164_63_6f_3c13f-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/V0KX>

https://aflow.org/p/A12B29_oC164_63_6f_3c13f-001

● Nb
● O



Prototype	Nb ₁₂ O ₂₉
AFLOW prototype label	A12B29_oC164_63_6f_3c13f-001
ICSD	24089

Pearson symbol	oC164
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	aflow --proto=A12B29_oC164_63_6f_3c13f-001 --params= <i>a, b/a, c/a, y1, y2, y3, y4, z4, y5, z5, y6, z6, y7, z7, y8, z8, y9, z9, y10, z10, y11, z11, y12, z12, y13, z13, y14, z14, y15, z15, y16, z16, y17, z17, y18, z18, y19, z19, y20, z20, y21, z21, y22, z22</i>

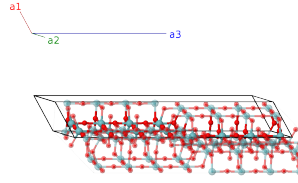
Other compounds with this structure

Ti₂Nb₁₀O₂₉

- Nb₁₂O₂₉ is known to exist in a least two phases (Norin, 1963; Norin, 1966):
 - a monoclinic phase and
 - an orthorhombic phase (this structure).
- (Wadsley, 1961) earlier found that both known phases of Ti₂Nb₁₂O₂₉ are isostructural with the corresponding Nb₁₂O₂₉ phase, but as the titanium and niobium atoms are alloyed on the same site we use the binary Nb₁₂O₂₉ as the prototype.
- (Norin, 1963) gives the structure of orthorhombic Nb₁₂O₂₉ in the *Amma* setting of space group #63. We used FINDSYM to transform it to the standard *Cmcm* setting.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B ₁	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	O I
B ₂	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	O I
B ₃	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	O II
B ₄	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	O II
B ₅	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	O III
B ₆	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	O III
B ₇	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	Nb I
B ₈	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Nb I
B ₉	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Nb I
B ₁₀	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8f)	Nb I
B ₁₁	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8f)	Nb II
B ₁₂	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Nb II
B ₁₃	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8f)	Nb II

$$\begin{aligned}
\mathbf{B}_{55} &= -y_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 &= & by_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}} & (8f) & \text{O X} \\
\mathbf{B}_{56} &= y_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 + \left(z_{16} + \frac{1}{2}\right) \mathbf{a}_3 &= & -by_{16} \hat{\mathbf{y}} + c \left(z_{16} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O X} \\
\mathbf{B}_{57} &= -y_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 - \left(z_{16} - \frac{1}{2}\right) \mathbf{a}_3 &= & by_{16} \hat{\mathbf{y}} - c \left(z_{16} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O X} \\
\mathbf{B}_{58} &= y_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 - z_{16} \mathbf{a}_3 &= & -by_{16} \hat{\mathbf{y}} - cz_{16} \hat{\mathbf{z}} & (8f) & \text{O X} \\
\mathbf{B}_{59} &= -y_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= & by_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (8f) & \text{O XI} \\
\mathbf{B}_{60} &= y_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 + \left(z_{17} + \frac{1}{2}\right) \mathbf{a}_3 &= & -by_{17} \hat{\mathbf{y}} + c \left(z_{17} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XI} \\
\mathbf{B}_{61} &= -y_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 - \left(z_{17} - \frac{1}{2}\right) \mathbf{a}_3 &= & by_{17} \hat{\mathbf{y}} - c \left(z_{17} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XI} \\
\mathbf{B}_{62} &= y_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3 &= & -by_{17} \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}} & (8f) & \text{O XI} \\
\mathbf{B}_{63} &= -y_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 &= & by_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (8f) & \text{O XII} \\
\mathbf{B}_{64} &= y_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 + \left(z_{18} + \frac{1}{2}\right) \mathbf{a}_3 &= & -by_{18} \hat{\mathbf{y}} + c \left(z_{18} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XII} \\
\mathbf{B}_{65} &= -y_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 - \left(z_{18} - \frac{1}{2}\right) \mathbf{a}_3 &= & by_{18} \hat{\mathbf{y}} - c \left(z_{18} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XII} \\
\mathbf{B}_{66} &= y_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3 &= & -by_{18} \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}} & (8f) & \text{O XII} \\
\mathbf{B}_{67} &= -y_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= & by_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} & (8f) & \text{O XIII} \\
\mathbf{B}_{68} &= y_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 &= & -by_{19} \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XIII} \\
\mathbf{B}_{69} &= -y_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 - \left(z_{19} - \frac{1}{2}\right) \mathbf{a}_3 &= & by_{19} \hat{\mathbf{y}} - c \left(z_{19} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XIII} \\
\mathbf{B}_{70} &= y_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3 &= & -by_{19} \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} & (8f) & \text{O XIII} \\
\mathbf{B}_{71} &= -y_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3 &= & by_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} & (8f) & \text{O XIV} \\
\mathbf{B}_{72} &= y_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 + \left(z_{20} + \frac{1}{2}\right) \mathbf{a}_3 &= & -by_{20} \hat{\mathbf{y}} + c \left(z_{20} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XIV} \\
\mathbf{B}_{73} &= -y_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 - \left(z_{20} - \frac{1}{2}\right) \mathbf{a}_3 &= & by_{20} \hat{\mathbf{y}} - c \left(z_{20} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XIV} \\
\mathbf{B}_{74} &= y_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 - z_{20} \mathbf{a}_3 &= & -by_{20} \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}} & (8f) & \text{O XIV} \\
\mathbf{B}_{75} &= -y_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3 &= & by_{21} \hat{\mathbf{y}} + cz_{21} \hat{\mathbf{z}} & (8f) & \text{O XV} \\
\mathbf{B}_{76} &= y_{21} \mathbf{a}_1 - y_{21} \mathbf{a}_2 + \left(z_{21} + \frac{1}{2}\right) \mathbf{a}_3 &= & -by_{21} \hat{\mathbf{y}} + c \left(z_{21} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XV} \\
\mathbf{B}_{77} &= -y_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 - \left(z_{21} - \frac{1}{2}\right) \mathbf{a}_3 &= & by_{21} \hat{\mathbf{y}} - c \left(z_{21} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XV} \\
\mathbf{B}_{78} &= y_{21} \mathbf{a}_1 - y_{21} \mathbf{a}_2 - z_{21} \mathbf{a}_3 &= & -by_{21} \hat{\mathbf{y}} - cz_{21} \hat{\mathbf{z}} & (8f) & \text{O XV} \\
\mathbf{B}_{79} &= -y_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3 &= & by_{22} \hat{\mathbf{y}} + cz_{22} \hat{\mathbf{z}} & (8f) & \text{O XVI} \\
\mathbf{B}_{80} &= y_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 + \left(z_{22} + \frac{1}{2}\right) \mathbf{a}_3 &= & -by_{22} \hat{\mathbf{y}} + c \left(z_{22} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XVI} \\
\mathbf{B}_{81} &= -y_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 - \left(z_{22} - \frac{1}{2}\right) \mathbf{a}_3 &= & by_{22} \hat{\mathbf{y}} - c \left(z_{22} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8f) & \text{O XVI} \\
\mathbf{B}_{82} &= y_{22} \mathbf{a}_1 - y_{22} \mathbf{a}_2 - z_{22} \mathbf{a}_3 &= & -by_{22} \hat{\mathbf{y}} - cz_{22} \hat{\mathbf{z}} & (8f) & \text{O XVI}
\end{aligned}$$

References

- [1] R. Norin, *The Crystal Structure of Nb₁₂O₂₉ (o-rh)*, Acta Chem. Scand. **17**, 1391–1404 (1963), doi:10.3891/acta.chem.scand.17-1391.
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