Monoclinic $Nb_{12}O_{29}$ Structure: A12B29_mC82_12_6i_a14i-001

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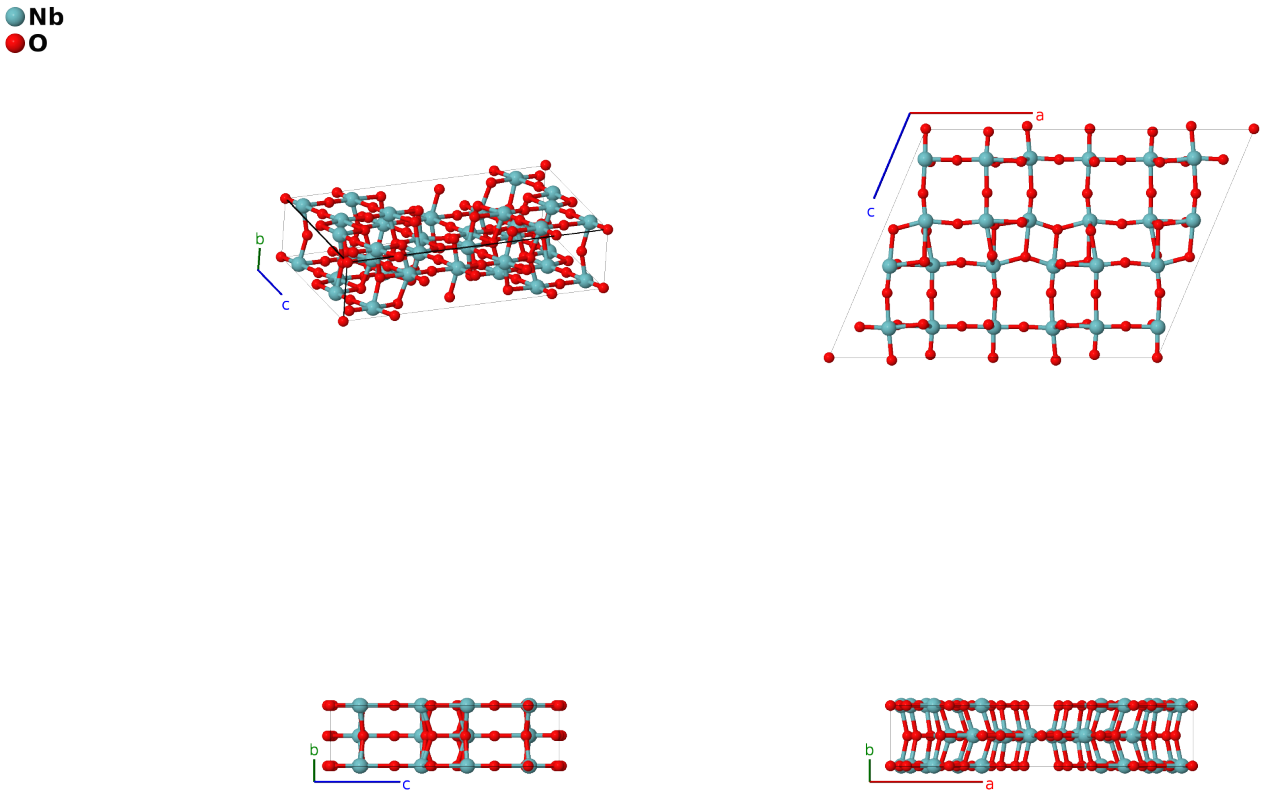


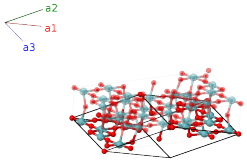
Prototype	$Nb_{12}O_{29}$
AFLOW prototype label	A12B29_mC82_12_6i_a14i-001
ICSD	24111
Pearson symbol	mC82
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A12B29_mC82_12_6i_a14i-001 --params=`$a, b/a, c/a, \beta, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}, x_{12}, z_{12}, x_{13}, z_{13}, x_{14}, z_{14}, x_{15}, z_{15}, x_{16}, z_{16}, x_{17}, z_{17}, x_{18}, z_{18}, x_{19}, z_{19}, x_{20}, z_{20}, x_{21}, z_{21}$

Other compounds with this structure
$Ti_2Nb_{10}O_{29}$

- $Nb_{12}O_{29}$ is known to exist in a least two phases (Norin, 1963; Norin, 1966):
  - a monoclinic phase (this structure) and
  - an orthorhombic phase.
- (Wadsley, 1961) earlier found that both known phases of $Ti_2Nb_{12}O_{29}$ are isostructural with the corresponding $Nb_{12}O_{29}$ phase, but as the titanium and niobium atoms are alloyed on the same site we use the binary $Nb_{12}O_{29}$ as the prototype.
- (Norin, 1966) gives the structure of orthorhombic $Nb_{12}O_{29}$ in the $A2/a$ setting of space group #15, with the origin at -1 on the a-glide plane. We when we checked this with FINDSYM we found that the structure could be placed in space group $C2/m$ #12 with a unit cell half that found by (Norin, 1966), and close to the dimensions of the cell found in (Wadsley, 1961) and (Norin, 1963).

Base-centered Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}\\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	O I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb II
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb II
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb III
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb III
$\mathbf{B_8}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb IV
$\mathbf{B_9}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb IV
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb V
$\mathbf{B_{11}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb V
$\mathbf{B_{12}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb VI
$\mathbf{B_{13}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4i)	Nb VI
$\mathbf{B_{14}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_{15}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B_{16}}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{17}}$	=	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} - cz_9\sin\beta\,\hat{\mathbf{z}}$	(4i)	O III
$\mathbf{B_{18}}$	=	$x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O IV
$\mathbf{B_{19}}$	=	$-x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} - cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O IV

$\mathbf{B_{20}}$	=	$x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O V
$\mathbf{B_{21}}$	=	$-x_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} - cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O V
$\mathbf{B_{22}}$	=	$x_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O VI
$\mathbf{B_{23}}$	=	$-x_{12}\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} - cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O VI
$\mathbf{B_{24}}$	=	$x_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O VII
$\mathbf{B_{25}}$	=	$-x_{13}\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$-(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} - cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O VII
$\mathbf{B_{26}}$	=	$x_{14}\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} + cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O VIII
$\mathbf{B_{27}}$	=	$-x_{14}\,\mathbf{a}_1 - x_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3$	=	$-(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} - cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O VIII
$\mathbf{B_{28}}$	=	$x_{15}\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$(ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} + cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O IX
$\mathbf{B_{29}}$	=	$-x_{15}\,\mathbf{a}_1 - x_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3$	=	$-(ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} - cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O IX
$\mathbf{B_{30}}$	=	$x_{16}\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$(ax_{16} + cz_{16}\cos\beta)\,\hat{\mathbf{x}} + cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O X
$\mathbf{B_{31}}$	=	$-x_{16}\,\mathbf{a}_1 - x_{16}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3$	=	$-(ax_{16} + cz_{16}\cos\beta)\,\hat{\mathbf{x}} - cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O X
$\mathbf{B_{32}}$	=	$x_{17}\,\mathbf{a}_1 + x_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3$	=	$(ax_{17} + cz_{17}\cos\beta)\,\hat{\mathbf{x}} + cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XI
$\mathbf{B_{33}}$	=	$-x_{17}\,\mathbf{a}_1 - x_{17}\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3$	=	$-(ax_{17} + cz_{17}\cos\beta)\,\hat{\mathbf{x}} - cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XI
$\mathbf{B_{34}}$	=	$x_{18}\,\mathbf{a}_1 + x_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3$	=	$(ax_{18} + cz_{18}\cos\beta)\,\hat{\mathbf{x}} + cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XII
$\mathbf{B_{35}}$	=	$-x_{18}\,\mathbf{a}_1 - x_{18}\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3$	=	$-(ax_{18} + cz_{18}\cos\beta)\,\hat{\mathbf{x}} - cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XII
$\mathbf{B_{36}}$	=	$x_{19}\,\mathbf{a}_1 + x_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3$	=	$(ax_{19} + cz_{19}\cos\beta)\,\hat{\mathbf{x}} + cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XIII
$\mathbf{B_{37}}$	=	$-x_{19}\,\mathbf{a}_1 - x_{19}\,\mathbf{a}_2 - z_{19}\,\mathbf{a}_3$	=	$-(ax_{19} + cz_{19}\cos\beta)\,\hat{\mathbf{x}} - cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XIII
$\mathbf{B_{38}}$	=	$x_{20}\,\mathbf{a}_1 + x_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3$	=	$(ax_{20} + cz_{20}\cos\beta)\,\hat{\mathbf{x}} + cz_{20}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XIV
$\mathbf{B_{39}}$	=	$-x_{20}\,\mathbf{a}_1 - x_{20}\,\mathbf{a}_2 - z_{20}\,\mathbf{a}_3$	=	$-(ax_{20} + cz_{20}\cos\beta)\,\hat{\mathbf{x}} - cz_{20}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XIV
$\mathbf{B_{40}}$	=	$x_{21}\,\mathbf{a}_1 + x_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3$	=	$(ax_{21} + cz_{21}\cos\beta)\,\hat{\mathbf{x}} + cz_{21}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XV
$\mathbf{B_{41}}$	=	$-x_{21}\,\mathbf{a}_1 - x_{21}\,\mathbf{a}_2 - z_{21}\,\mathbf{a}_3$	=	$-(ax_{21} + cz_{21}\cos\beta)\,\hat{\mathbf{x}} - cz_{21}\sin\beta\,\hat{\mathbf{z}}$	(4i)	O XV

References

[1] R. Norin, *The Crystal Structure of $Nb_{12}O_{29}$ (o-rh)*, Acta Chem. Scand. **17**, 1391–1404 (1963), doi:10.3891/acta.chem.scand.17-1391.

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[3] A. D. Wadsley, *Mixed oxides of titanium and niobium. II. The crystal structures of the dimorphic forms $Ti_2Nb_{10}O_{29}$*, Acta Cryst. **14**, 664–670 (1961), doi:10.1107/S0365110X6100200X.