

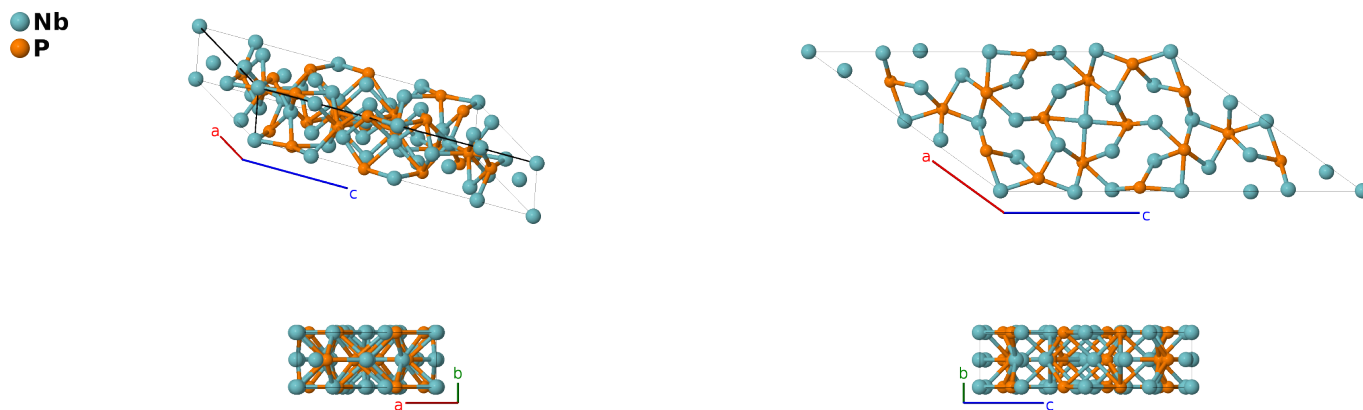
Nb₇P₄ Structure:

A7B4_mC44_12_ac6i_4i-001

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<https://aflow.org/p/EWT8>

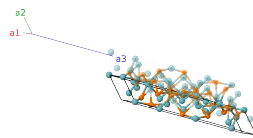
https://aflow.org/p/A7B4_mC44_12_ac6i_4i-001



Prototype	Nb ₇ P ₄
AFLOW prototype label	A7B4_mC44_12_ac6i_4i-001
ICSD	41238
Pearson symbol	mC44
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	aflow --proto=A7B4_mC44_12_ac6i_4i-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , β , <i>x</i> ₃ , <i>z</i> ₃ , <i>x</i> ₄ , <i>z</i> ₄ , <i>x</i> ₅ , <i>z</i> ₅ , <i>x</i> ₆ , <i>z</i> ₆ , <i>x</i> ₇ , <i>z</i> ₇ , <i>x</i> ₈ , <i>z</i> ₈ , <i>x</i> ₉ , <i>z</i> ₉ , <i>x</i> ₁₀ , <i>z</i> ₁₀ , <i>x</i> ₁₁ , <i>z</i> ₁₁ , <i>x</i> ₁₂ , <i>z</i> ₁₂

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(2a) Nb I
\mathbf{B}_2	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(2c) Nb II
\mathbf{B}_3	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Nb III

\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 III
\mathbf{B}_5	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	$(4i)$	Nb IV
\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 IV
\mathbf{B}_7	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	$(4i)$	Nb V
\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 V
\mathbf{B}_9	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	$(4i)$	Nb VI
\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 VI
\mathbf{B}_{11}	$= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	$(4i)$	Nb VII
\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 VII
\mathbf{B}_{13}	$= x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	$(4i)$	Nb VIII
\mathbf{B}_{14}	$= -x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}}$	$(4i)$	Nb VIII
\mathbf{B}_{15}	$= x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}}$	$(4i)$	P I
\mathbf{B}_{16}	$= -x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - cz_9 \sin \beta \hat{\mathbf{z}}$	$(4i)$	P I
\mathbf{B}_{17}	$= x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	$(4i)$	P II
\mathbf{B}_{18}	$= -x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	$(4i)$	P II
\mathbf{B}_{19}	$= x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	$(4i)$	P III
\mathbf{B}_{20}	$= -x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	$(4i)$	P III
\mathbf{B}_{21}	$= x_{12} \mathbf{a}_1 + x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	$(4i)$	P IV
\mathbf{B}_{22}	$= -x_{12} \mathbf{a}_1 - x_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - cz_{12} \sin \beta \hat{\mathbf{z}}$	$(4i)$	P IV

References

- [1] S. Rundqvist, *The Crystal Structure of Nb₇P₄*, Acta Chem. Scand. **20**, 2427–2434 (1966), doi:10.3891/acta.chem.scand.20-2427.