

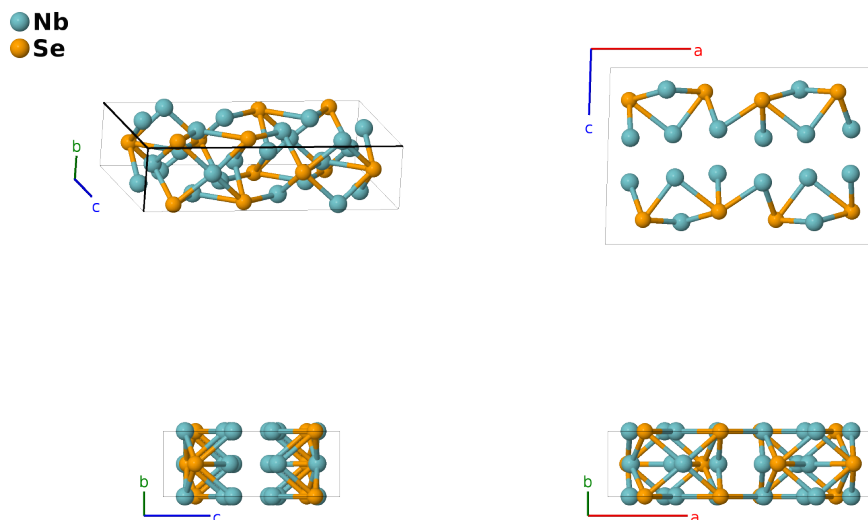
Nb₂Se Structure:

A2B_mC24_12_4i_2i-004

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<https://aflow.org/p/2691>

https://aflow.org/p/A2B_mC24_12_4i_2i-004



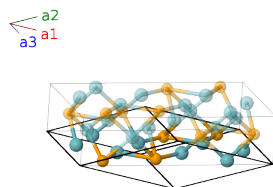
Prototype	Nb ₂ Se
AFLOW prototype label	A2B_mC24_12_4i_2i-004
ICSD	26183
Pearson symbol	mC24
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	aflow --proto=A2B_mC24_12_4i_2i-004 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , β , <i>x</i> ₁ , <i>z</i> ₁ , <i>x</i> ₂ , <i>z</i> ₂ , <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

Other compounds with this structure

Hf₂Se

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	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4i)	Nb I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(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 II
\mathbf{B}_4	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	Nb 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 III
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Nb III
\mathbf{B}_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 IV
\mathbf{B}_8	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	Nb IV
\mathbf{B}_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)	Se I
\mathbf{B}_{10}	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	Se I
\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)	Se II
\mathbf{B}_{12}	$= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	Se II

References

- [1] B. R. Conard, L. J. Norrby, and H. F. Franzen, *The crystal structure of Nb₂Se*, Acta Crystallogr. Sect. B **25**, 1729–1736 (1969), doi:10.1107/S0567740869004663.