

NbSe₃ Structure:

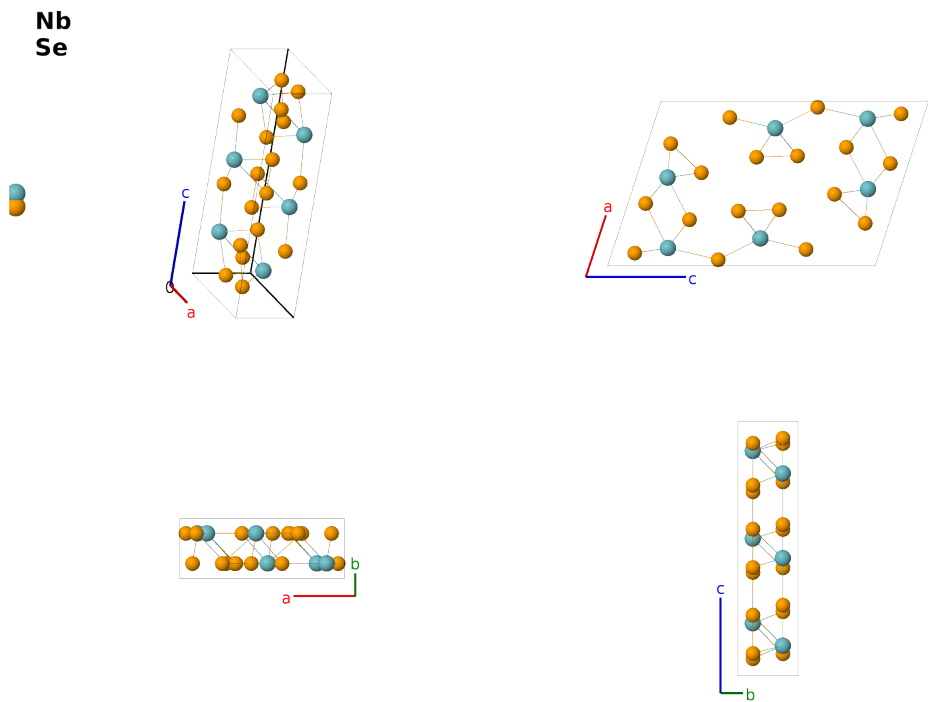
AB3_mP24_11_3e_9e-001

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- 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/4LKF>

https://aflow.org/prototype-encyclopedia/AB3_mP24_11_3e_9e-001



Prototype	NbSe ₃
AFLOW prototype label	AB3_mP24_11_3e_9e-001
ICSD	76579
CCDC	1637138
Pearson symbol	mP24
Space group number	11
Space group symbol	$P2_1/m$
AFLOW prototype command	<pre>aflow --proto=AB3_mP24_11_3e_9e-001 --params=a,b/a,c/a,β,x_1,z_1,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}</pre>

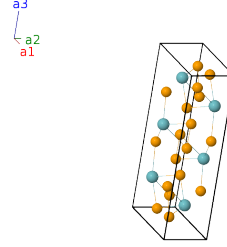
Other compounds with this structure

TaS₃

- We use the structure data taken by (Hodeau, 1978) at 100K.

Simple Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Nb I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2e)	Nb I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Nb II
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2e)	Nb II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Nb III
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2e)	Nb III
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Se I
$\mathbf{B}_8$	$-x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2e)	Se I
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	Se II
$\mathbf{B}_{10}$	$-x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2e)	Se II
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	Se III
$\mathbf{B}_{12}$	$-x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2e)	Se III
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2e)	Se IV
$\mathbf{B}_{14}$	$-x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(2e)	Se IV
$\mathbf{B}_{15}$	$x_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2e)	Se V
$\mathbf{B}_{16}$	$-x_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(2e)	Se V
$\mathbf{B}_{17}$	$x_9 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2e)	Se VI
$\mathbf{B}_{18}$	$-x_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3$	=	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(2e)	Se VI
$\mathbf{B}_{19}$	$x_{10} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2e)	Se VII
$\mathbf{B}_{20}$	$-x_{10} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	=	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(2e)	Se VII
$\mathbf{B}_{21}$	$x_{11} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(2e)	Se VIII
$\mathbf{B}_{22}$	$-x_{11} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	=	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(2e)	Se VIII
$\mathbf{B}_{23}$	$x_{12} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	=	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(2e)	Se IX
$\mathbf{B}_{24}$	$-x_{12} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	=	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_{12} \sin \beta \hat{\mathbf{z}}$	(2e)	Se IX

References

- [1] J. L. Hodeau, M. Marezio, C. Roucau, R. Ayroles, A. Meerschaut, J. Rouxel, and P. Monceau, *Charge-density waves in NbSe₃ at 145K: crystal structures, X-ray and electron diffraction studies*, J. Phys. C: Solid State Phys. **11**, 4117–4134 (1978), doi:10.1088/0022-3719/11/20/009.

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