Low Temperature NbSe$_2$ Structure: AB2_hP24_194_bh_fk-001

https://aflow.org/p/YM9E

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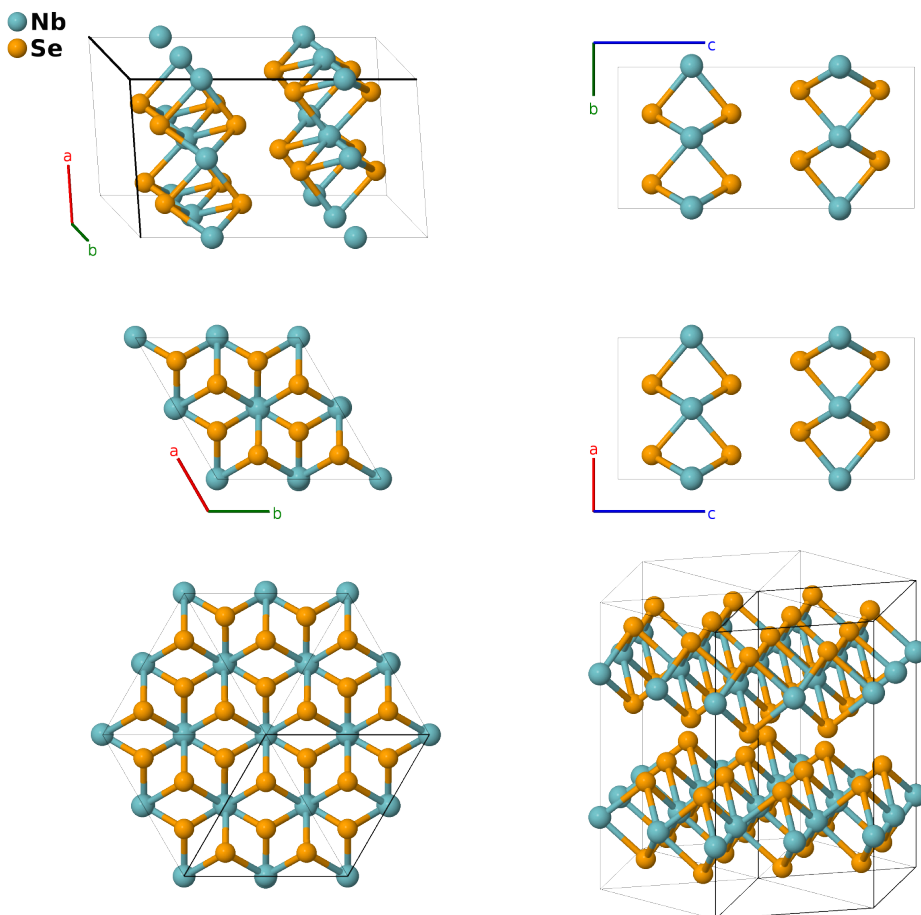
Prototype	NbSe$_2$
AFLOW prototype label	AB2_hP24_194_bh_fk-001
ICSD	16305
Pearson symbol	hP24
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	aflow --proto=AB2_hP24_194_bh_fk-001 --params=$a, c/a, z_2, x_3, x_4, z_4$

- NbSe$_2$ is in the high temperature NbS$_2$ structure above 40K. Below 40K the primitive cell doubles in the a and b directions, and the niobium atoms are no longer equivalent, giving this structure.

- The data for this structure was taken at 15K.

Hexagonal primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
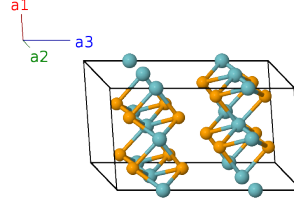
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2b)	Nb I
$\mathbf{B_2}$	$=$	$\tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2b)	Nb I
$\mathbf{B_3}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B_4}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \left(z_2 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B_5}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B_6}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} - \left(z_2 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_2 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(4f)	Se I
$\mathbf{B_7}$	$=$	$x_3\,\mathbf{a_1} + 2x_3\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_3\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb II
$\mathbf{B_8}$	$=$	$-2x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_3\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb II
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$-\sqrt{3}ax_3\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb II
$\mathbf{B_{10}}$	$=$	$-x_3\,\mathbf{a_1} - 2x_3\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_3\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb II
$\mathbf{B_{11}}$	$=$	$2x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_3\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb II
$\mathbf{B_{12}}$	$=$	$-x_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\sqrt{3}ax_3\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Nb II
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a_1} + 2x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{14}}$	$=$	$-2x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{15}}$	$=$	$x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{16}}$	$=$	$-x_4\,\mathbf{a_1} - 2x_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{17}}$	$=$	$2x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{18}}$	$=$	$-x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\sqrt{3}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{19}}$	$=$	$2x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{20}}$	$=$	$-x_4\,\mathbf{a_1} - 2x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{21}}$	$=$	$-x_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$\sqrt{3}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{22}}$	$=$	$-2x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{23}}$	$=$	$x_4\,\mathbf{a_1} + 2x_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_4\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12k)	Se II
$\mathbf{B_{24}}$	$=$	$x_4\,\mathbf{a_1} - x_4\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12k)	Se II

References

[1] M. Marezio, P. D. Dernier, A. Menth, and J. G. W. Hull, *The Crystal Structure of NbSe₂ at °15K*, J. Solid State Chem. **4**, 425–429 (1972), doi:10.1016/0022-4596(72)90158-2.