

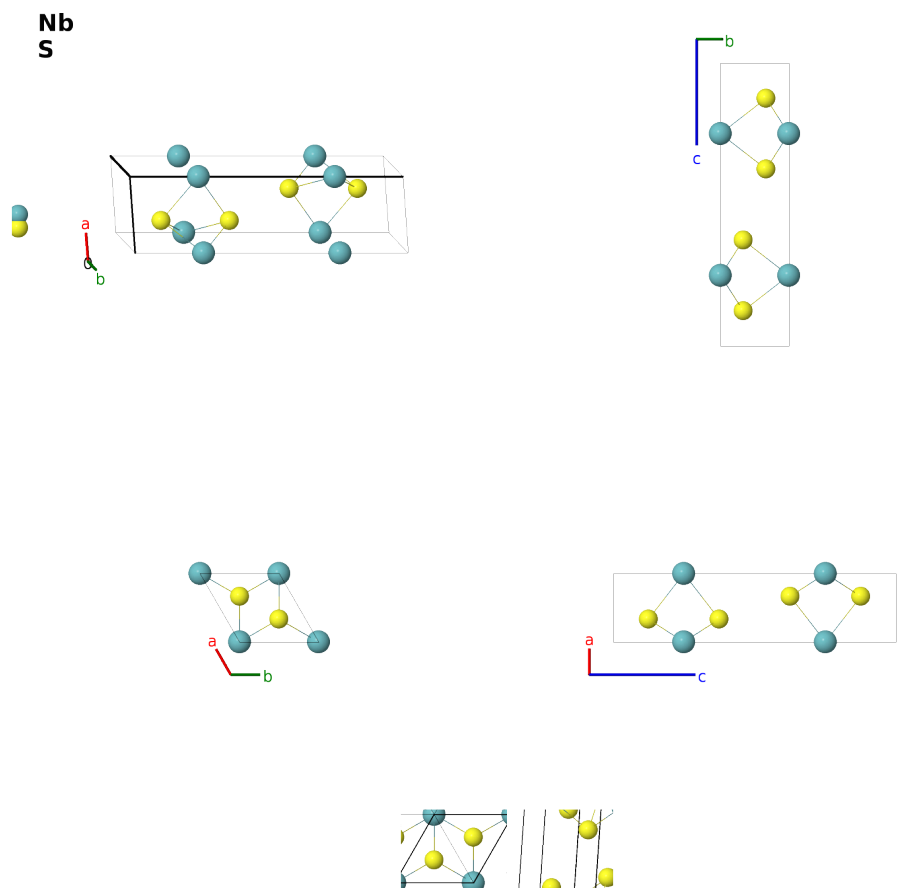
Hexagonal High-Temperature NbS₂ Structure: AB2_hP6_194_b-f-002

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<https://aflow.org/prototype-encyclopedia/Z5TL>

https://aflow.org/prototype-encyclopedia/AB2_hP6_194_b-f-002



Prototype	NbS ₂
AFLOW prototype label	AB2_hP6_194_b-f-002
ICSD	43697
CCDC	1613169
Pearson symbol	hP6
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=AB2_hP6_194_b-f-002</code> <code>--params=a, c/a, z₂</code>

Other compounds with this structure

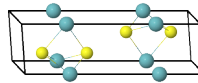
NbSe₂

- This hexagonal structure is stable from 850°C to 1050°C. Below 800°C NbS₂ takes on the rhombohedral MoS₂ structure.
- CaIn₂ and hexagonal NbS₂ have the same AFLOW label, AB2_hP6_194_b.f. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$





Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}c\hat{\mathbf{z}}$	(2b)	Nb I
$\mathbf{B}_2$	$= \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}c\hat{\mathbf{z}}$	(2b)	Nb I
$\mathbf{B}_3$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 + z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B}_4$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + (z_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + c(z_2 + \frac{1}{2})\hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B}_5$	$= \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 - z_2\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - cz_2\hat{\mathbf{z}}$	(4f)	S I
$\mathbf{B}_6$	$= \frac{1}{3}\mathbf{a}_1 + \frac{2}{3}\mathbf{a}_2 - (z_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} - c(z_2 - \frac{1}{2})\hat{\mathbf{z}}$	(4f)	S I

References

- [1] F. Jellinek, G. Brauer, and H. Müller, *Molybdenum and Niobium Sulphides*, Nature **185**, 376–377 (1960), doi:10.1038/185376a0.

Found in

- [1] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. R., S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.

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