

Low Temperature Nb_{1-x}S Structure:

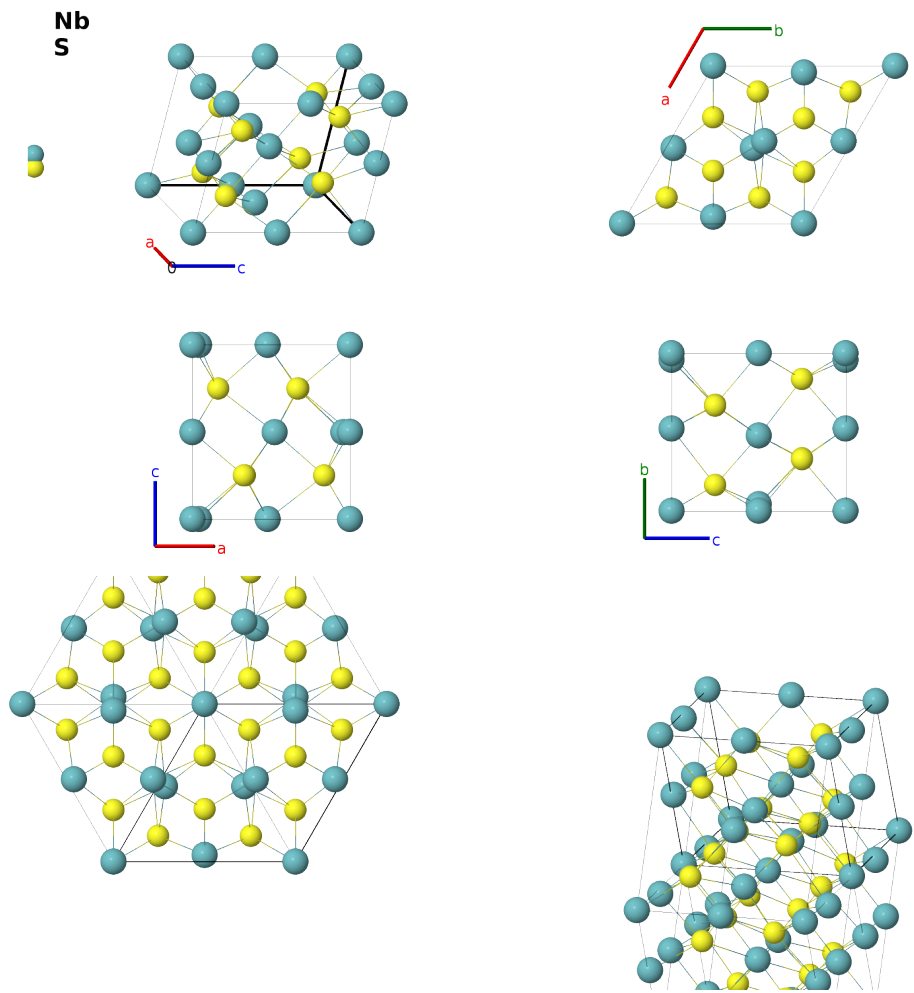
AB_hP16_186_ac_bc-002

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<https://aflow.org/prototype-encyclopedia/VW80>

https://aflow.org/prototype-encyclopedia/AB_hP16_186_ac_bc-002



Prototype	NbS
AFLOW prototype label	AB_hP16_186_ac_bc-002
ICSD	15679
CCDC	1596386
Pearson symbol	hP16
Space group number	186
Space group symbol	$P6_3mc$

AFLOW prototype command `aflow --proto=AB_hP16_186_ac_bc-002`
 `--params=a, c/a, z1, z2, x3, z3, x4, z4`

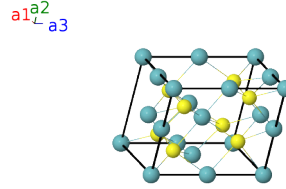
Other compounds with this structure

MoN

- This is the low-temperature structure of sulfur-rich NbS, tempered at $\approx 650^\circ\text{C}$ from the high-temperature phase, which takes on the orthorhombic MnP (*B31*) structure. The metal-rich form, Nb_{1+x}S, is in the NiAs (*B8₁*) structure.
- (Kadijk, 1969) give the occupancy of the Nb (2a) site as 68%, making the stoichiometry of this sample Nb_{0.92}S.
- Space group *P6₃mc*#186 does not define the origin of the *z*-axis. Here we follow (Kadijk, 1969) and set *z*₁ = 0 for the Nb-I site.
- While (Kadijk, 1969) set *x*₄=0.1634 for the S II site, the ICSD entry uses *x*₄=-0.1634. Using the former value gives unusual voids in the crystal structure which are not found with the later value. Accordingly we use the ICSD value -0.1634.

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
B₁	$z_1 \mathbf{a}_3$	=	$cz_1 \hat{\mathbf{z}}$	(2a)	Nb I
B₂	$(z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Nb I
B₃	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2b)	S I
B₄	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	S I
B₅	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Nb II
B₆	$x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Nb II
B₇	$-2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	Nb II
B₈	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$\sqrt{3}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Nb II
B₉	$-x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Nb II
B₁₀	$2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	Nb II
B₁₁	$x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$-\sqrt{3}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	S II
B₁₂	$x_4 \mathbf{a}_1 + 2x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	S II
B₁₃	$-2x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	S II
B₁₄	$-x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$\sqrt{3}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	S II
B₁₅	$-x_4 \mathbf{a}_1 - 2x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	S II
B₁₆	$2x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{3}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(6c)	S II

References

- [1] F. Kadijk and F. Jellinek, *The System Niobium-Sulfur*, J. Less-Common Met. **19**, 421–430 (1969), doi:10.1016/0022-5088(69)90187-8.

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

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