

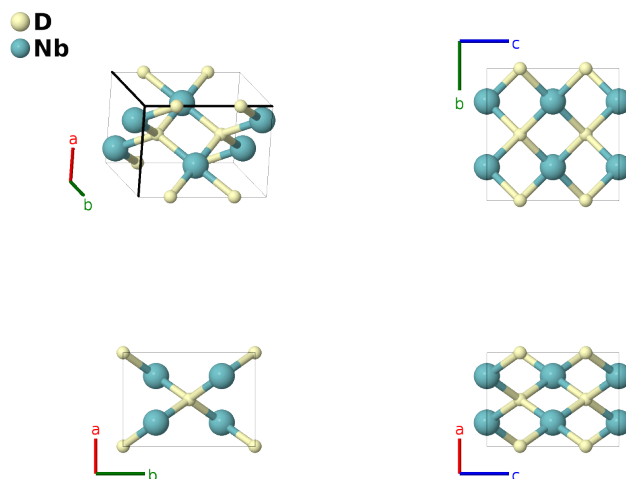
NbD Structure:

AB_oC8_66_a_e-001

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<https://aflow.org/p/087H>

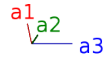
https://aflow.org/p/AB_oC8.66_a_e-001



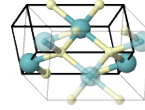
Prototype	HNb
AFLOW prototype label	AB_oC8_66_a_e-001
ICSD	71093
Pearson symbol	oC8
Space group number	66
Space group symbol	<i>Cccm</i>
AFLOW prototype command	<code>aflow --proto=AB_oC8_66_a_e-001 --params=a,b/a,c/a</code>

- The deuterium sites in this structure have 5% vacancies.
- (Somenkov, 1968) do not actually give the lattice constants for this structure. They are inferred from the Nb-H and H-H distances given for NbH_{0.85}.
- (Somenkov, 1968) described this structure in space group *Pnnn* #48, but the positions given actually for the conventional cell of space group *Cccm* #66. (Cenzual, 1991)

Base-centered Orthorhombic primitive vectors



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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1 =$	$\frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(4a)	D I
$\mathbf{B}_2 =$	$\frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(4a)	D I
$\mathbf{B}_3 =$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(4e)	Nb I
$\mathbf{B}_4 =$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4e)	Nb I

References

- [1] V. A. Somenkov, A. V. Gurskaya, M. G. Zemlyanov, M. E. Kost, N. A. Chernoplekov, and A. A. Chertkov, *Neutron Scattering Study of Structure and Phase Transitions of Niobium Hydrides and Deuterides*, Sov. Phys. – Solid State **10**, 1076–1082 (1968).

Found in

- [1] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.