NbD Structure: AB_oC8_66_a_e-001

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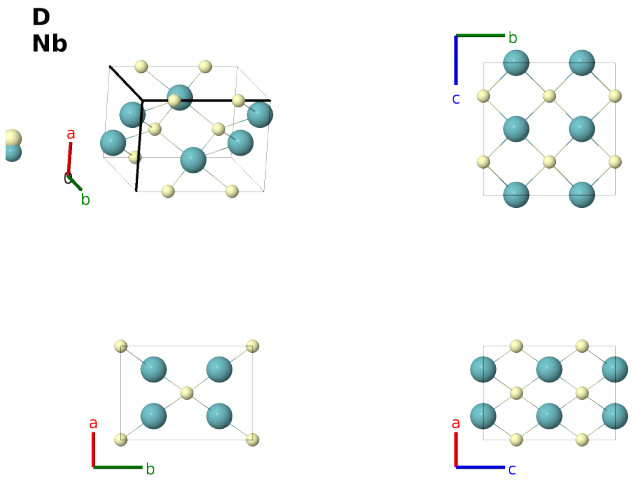
https://aflow.org/prototype-encyclopedia/087H

https://aflow.org/prototype-encyclopedia/AB_oC8_66_a_e-001

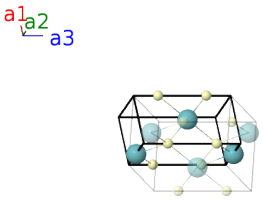


Prototype	HNb
AFLOW prototype label	AB_oC8_66_a_e-001
ICSD	71093
CCDC	1632002
Pearson symbol	oC8
Space group number	66
Space group symbol	$Cccm$
AFLOW prototype command	`aflow --proto=AB_oC8_66_a_e-001 --params=`$a, b/a, c/a$

- 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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.

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