

NbO Structure:

AB_cP6_221_c-d-001

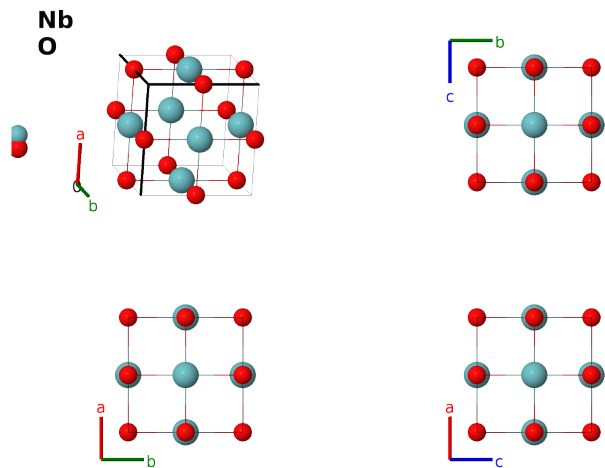
This structure previously used the label(s) **AB_cP6_221_c-d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/H75X>

https://aflow.org/prototype-encyclopedia/AB_cP6_221_c-d-001



Prototype	NbO
AFLOW prototype label	AB_cP6_221_c-d-001
ICSD	14338
CCDC	1595724
Pearson symbol	cP6
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB_cP6_221_c-d-001 --params=a</code>

Other compounds with this structure

NaS, KS

- This is the NaCl (*B1*) structure with 25% ordered vacancies on both the Na and Cl sites.
- At times we incorrectly referred to this structure as NaO.

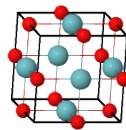
Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$

$\mathbf{a}_1$
 $\mathbf{a}_2$
 $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Nb I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c)	Nb I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(3c)	Nb I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(3d)	O I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(3d)	O I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(3d)	O I

References

- [1] A. L. Bowman, T. C. Wallace, J. L. Yarnell, and R. G. Wenzel, *The crystal structure of niobium monoxide*, *Acta Cryst.* **21**, 843 (1966), doi:10.1107/S0365110X66004043.

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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