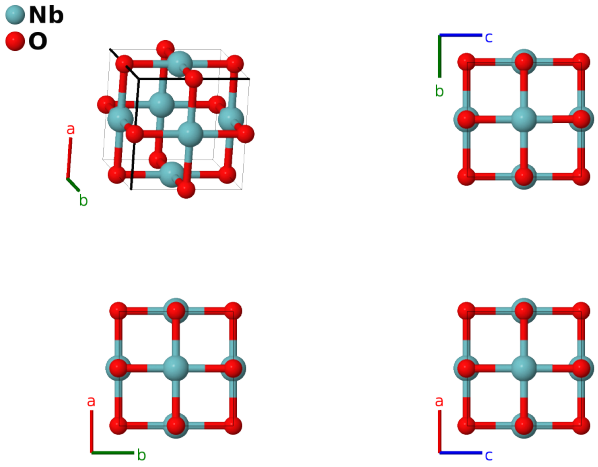
NbO Structure: AB_cP6_221_c_d-001

This structure originally had the label `AB_cP6_221_c_d`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/H75X

https://aflow.org/p/AB_cP6_221_c_d-001



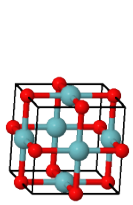
Prototype	NbO
AFLOW prototype label	AB_cP6_221_c_d-001
ICSD	14338
Pearson symbol	cP6
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_cP6_221_c_d-001 --params=`a

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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



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.