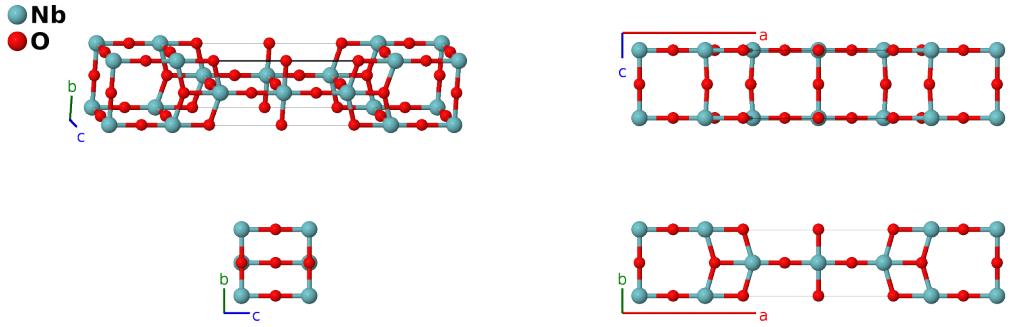
Nb_3O_7F Structure: A3B8_oC22_65_bg_ac2gh-001

This structure originally had the label `A3B8_oC22_65_ag_bd2gh`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/YUGM

https://aflow.org/p/A3B8_oC22_65_bg_ac2gh-001



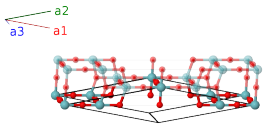
Prototype	FNb_3O_7
AFLOW prototype label	A3B8_oC22_65_bg_ac2gh-001
ICSD	28461
Pearson symbol	oC22
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=A3B8_oC22_65_bg_ac2gh-001 --params=`$a, b/a, c/a, x_4, x_5, x_6, x_7$

Other compounds with this structure
$Nb_3O_7(OH)$

- (Andersson, 1964) was not able to distinguish between oxygen and fluorine, so it is assumed that the fluorine atoms (or OH radicals) are distributed randomly on the oxygen sites. We follow Andersson and label all the sites as oxygen.

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
$\mathbf{B_1}$	=	0	=	0	(2a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Nb I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	O II
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}}$	(4g)	Nb II
$\mathbf{B_5}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}$	(4g)	Nb II
$\mathbf{B_6}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}}$	(4g)	O III
$\mathbf{B_7}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}}$	(4g)	O III
$\mathbf{B_8}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}}$	(4g)	O IV
$\mathbf{B_9}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}}$	(4g)	O IV
$\mathbf{B_{10}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O V
$\mathbf{B_{11}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	O V

References

[1] S. Andersson, *The Crystal Structure of Nb_3O_7F*, Acta Chem. Scand. **18**, 2339–2344 (1964), doi:10.3891/acta.chem.scand.18-2339.