$NaNbO_3$ $P4/mbm$ Lueshite Perovskite Structure: ABC3_tP10_127_c_a_bg-001

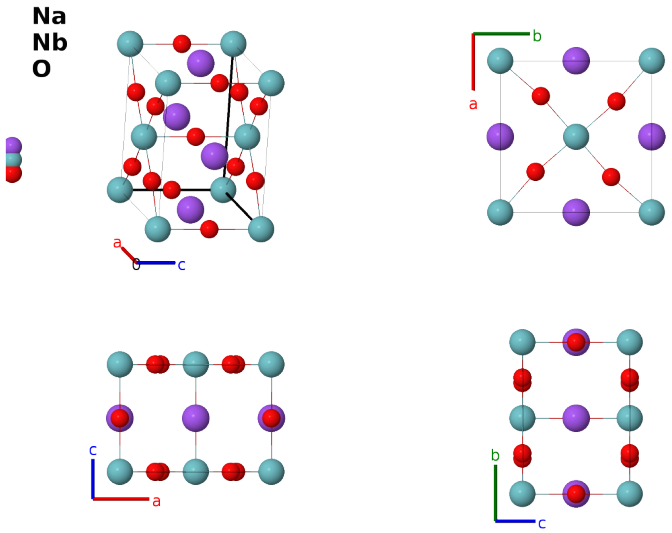
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/G9EC

https://aflow.org/prototype-encyclopedia/ABC3_tP10_127_c_a_bg-001



Prototype	$NaNbO_3$
AFLOW prototype label	ABC3_tP10_127_c_a_bg-001
ICSD	192406
CCDC	1701291
Pearson symbol	tP10
Space group number	127
Space group symbol	$P4/mbm$
AFLOW prototype command	`aflow --proto=ABC3_tP10_127_c_a_bg-001 --params=`$a, c/a, x_4$

Other compounds with this structure
$AgTaO_3$, $CsDyBr_3$, $CuKF_3$, $NaMgF_3$, $NaTaO_3$, $SrNbO_3$

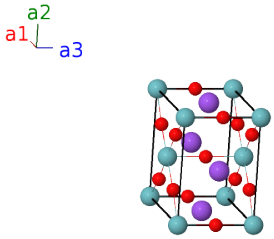
- As with most perovskites, $NaNbO_3$ (Lueshite) exists in a variety of forms depending on temperature and composition. Many of these phases are identified in (Mitchell, 2014). There is no consistent naming scheme that we are aware of, so we list the structures by space group. All the structure are identified in (Mitchell, 2014) unless otherwise noted. The paper does not give phase boundaries, so we will only indicate the temperatures at which the measurements were made.

- Synthetic Lueshite in orthorhombic space group *Pbcm* #57.
- (Mitchell, 2014) find naturally occurring Lueshite in the *Pnma* $CaTiO_3$ phase.
- (Vousden, 1951) found a ferroelectric Lueshite in space group $P222_1$ #17.
- At 575 and 600°C Lueshite is in the base-centered orthorhombic space group *Cmcm* #63.
- At 625°C, Lueshite is in the orthorhombic space group $P4/mbm$ #127. (this structure)
- At 650 and 675°C, and presumably at higher temperatures, $NaNbO_3$ is in the cubic perovskite ($E2_1$) structure.

- We use the data taken at 625°C.
- The similar structures are listed in the form ABC_3, where the "A" species are on the (2c) sites, the "B" species on the (2a) site, and the "C" species on the (2b), and (4g) sites. The A and B sites are often alloyed.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Nb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2a)	Nb I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Na I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Na I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_9}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(4g)	O II
$\mathbf{B_{10}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(4g)	O II

References

[1] R. H. Mitchell, P. C. Burns, K. S. Knight, C. J. Howard, and A. R. Chakhmouradian, *Observations on the crystal structures of lueshite*, Phys. Chem. Minerals **41**, 393–401 (2014), doi:10.1007/s00269-014-0657-1.

[2] P. Vousden, *The Structure of Ferroelectric Sodium Niobate at Room Temperature*, Acta Cryst. **4**, 545–551 (1951), doi:10.1107/S0365110X51001768.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).