Ferroelectric $NaNbO_3$ $P222_1$ Lueshite Perovskite Structure: ABC3_oP40_17_abcd_2e_abcd4e-001

This structure previously used the label(s) `ABC3_oP40_17_abcd_2e_abcd4e`. Calls to these addresses will be redirected here.

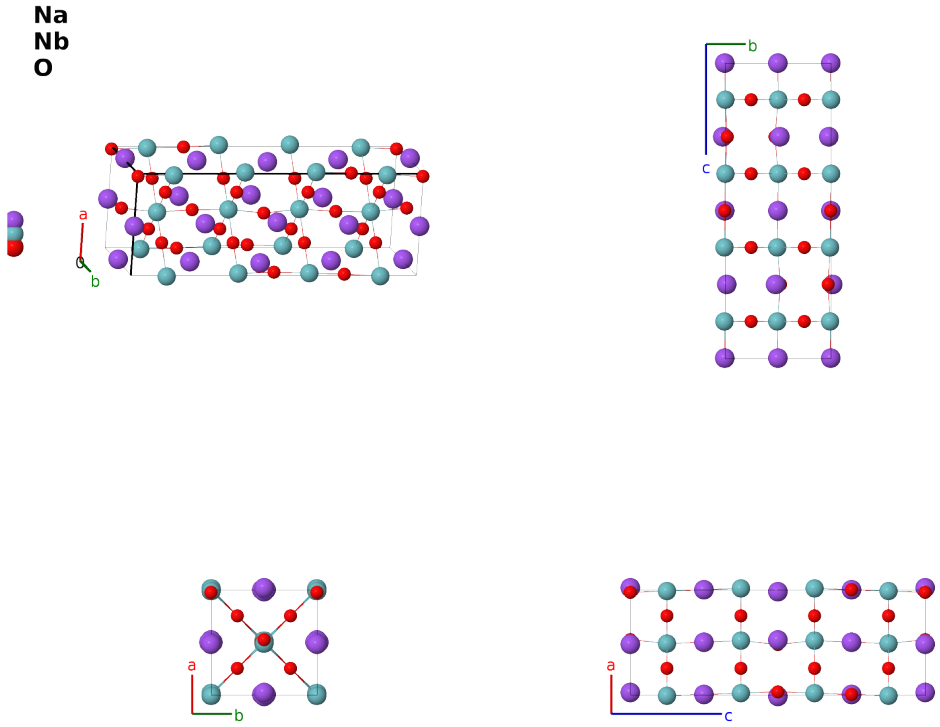
Cite this page as:

- 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/D6BJ

https://aflow.org/prototype-encyclopedia/ABC3_oP40_17_abcd_2e_abcd4e-001



Prototype	$NaNbO_3$
AFLOW prototype label	ABC3_oP40_17_abcd_2e_abcd4e-001
ICSD	76432
CCDC	1637027
Pearson symbol	oP40
Space group number	17
Space group symbol	$P222_1$

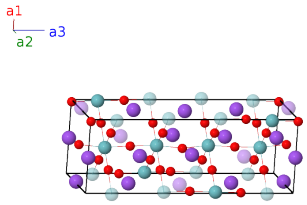
AFLOW prototype command `aflow --proto=ABC3_oP40_17_abcd_2e_abcd4e-001 --params=`$a, b/a, c/a, x_1, x_2, x_3, x_4, y_5, y_6, y_7, y_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}$

Other compounds with this structure
$BaCuO_{2+\delta}$ (HP)

- 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 $P222_1$. (this structure) #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.
  - At 650 and 675°C, and presumably at higher temperatures, $NaNbO_3$ is in the cubic perovskite ($E2_1$) structure.
- (Downs, 2003) identifies this as a "possible polymorph of lueshite."
- If the aflow parameters are set to `--params=`$a, 1, \sqrt{8}, 1/2, 0, 0, 1/2, 1/2, 0, 0, 1/2, 0, 0, 3/8, 1/2, 1/2, 3/8, 1/4, 1/4, 3/8, 3/4, 1/4, 3/8, 1/4, 3/4, 3/8, 3/4, 3/4, 3/8$ then this structure is equivalent to cubic perovskite $E2_1$.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$ax_1\,\hat{\mathbf{x}}$	(2a)	Na I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}}$	(2a)	O I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	Na II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Na II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(2b)	O II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_9}$	=	$y_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Na III

$\mathbf{B_{10}}$	=	$-y_5\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Na III
$\mathbf{B_{11}}$	=	$y_6\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	O III
$\mathbf{B_{12}}$	=	$-y_6\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	O III
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2d)	Na IV
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2d)	Na IV
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2d)	O IV
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2d)	O IV
$\mathbf{B_{17}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4e)	Nb I
$\mathbf{B_{18}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Nb I
$\mathbf{B_{19}}$	=	$-x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Nb I
$\mathbf{B_{20}}$	=	$x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(4e)	Nb I
$\mathbf{B_{21}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(4e)	Nb II
$\mathbf{B_{22}}$	=	$-x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Nb II
$\mathbf{B_{23}}$	=	$-x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Nb II
$\mathbf{B_{24}}$	=	$x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(4e)	Nb II
$\mathbf{B_{25}}$	=	$x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(4e)	O V
$\mathbf{B_{26}}$	=	$-x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O V
$\mathbf{B_{27}}$	=	$-x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O V
$\mathbf{B_{28}}$	=	$x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(4e)	O V
$\mathbf{B_{29}}$	=	$x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(4e)	O VI
$\mathbf{B_{30}}$	=	$-x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + c\left(z_{12} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O VI
$\mathbf{B_{31}}$	=	$-x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 - \left(z_{12} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} - c\left(z_{12} - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O VI
$\mathbf{B_{32}}$	=	$x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} - cz_{12}\,\hat{\mathbf{z}}$	(4e)	O VI
$\mathbf{B_{33}}$	=	$x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B_{34}}$	=	$-x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} + c\left(z_{13} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B_{35}}$	=	$-x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 - \left(z_{13} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}} + by_{13}\,\hat{\mathbf{y}} - c\left(z_{13} - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B_{36}}$	=	$x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}} - by_{13}\,\hat{\mathbf{y}} - cz_{13}\,\hat{\mathbf{z}}$	(4e)	O VII
$\mathbf{B_{37}}$	=	$x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$ax_{14}\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B_{38}}$	=	$-x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 + \left(z_{14} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{14}\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} + c\left(z_{14} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B_{39}}$	=	$-x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 - \left(z_{14} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{14}\,\hat{\mathbf{x}} + by_{14}\,\hat{\mathbf{y}} - c\left(z_{14} - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	O VIII
$\mathbf{B_{40}}$	=	$x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3$	=	$ax_{14}\,\hat{\mathbf{x}} - by_{14}\,\hat{\mathbf{y}} - cz_{14}\,\hat{\mathbf{z}}$	(4e)	O VIII

References

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

[2] 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.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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.