

NaNbO₃ *Pbcm* Lueshite Perovskite Structure: ABC3_oP40_57_cd_e_cd2e-001

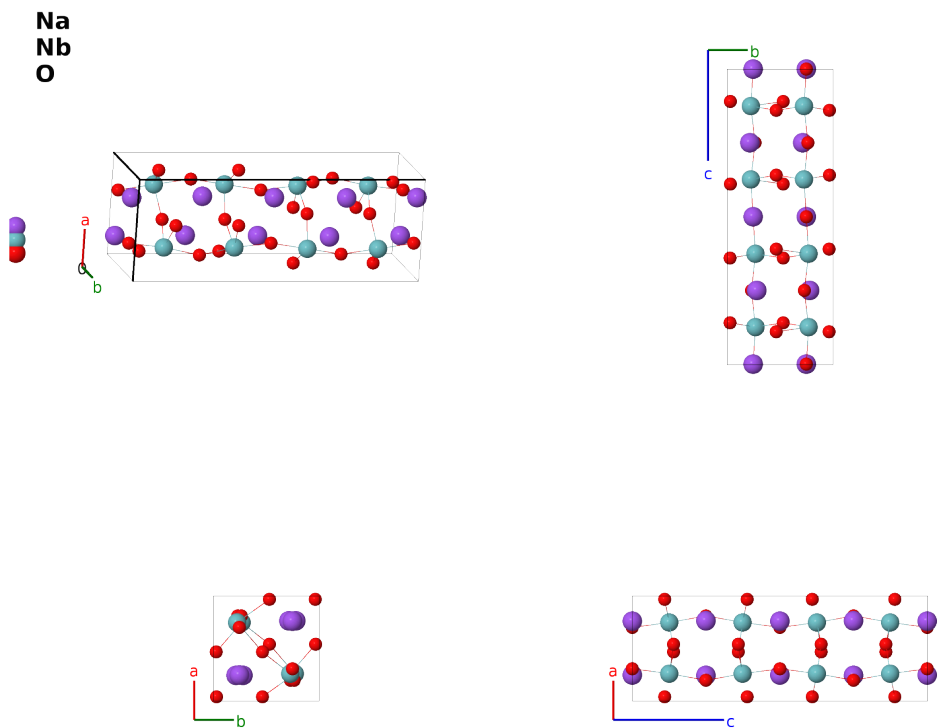
This structure previously used the label(s) **ABC3_oP40_57_cd_e_cd2e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/1JM3>

https://aflow.org/prototype-encyclopedia/ABC3_oP40_57_cd_e_cd2e-001



Prototype	NaNbO ₃
AFLOW prototype label	ABC3_oP40_57_cd_e_cd2e-001
Mineral name	lueshite
ICSD	23239
CCDC	1599371
Pearson symbol	oP40
Space group number	57
Space group symbol	<i>Pbcm</i>

AFLOW prototype command `aflow --proto=ABC3_oP40_57_cd_e_cd2e-001`
 `--params=a, b/a, c/a, x1, x2, x3, y3, x4, y4, x5, y5, z5, x6, y6, z6, x7, y7, z7`

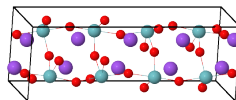
Other compounds with this structure

AgNbO₃, SrTiO₃, NaNb_{1-x}Ti_xO₃

- As with most perovskites, NaNbO₃ (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. (this structure)
 - (Mitchell, 2014) find naturally occurring Lueshite in the *Pnma* CaTiO₃ 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.
 - At 650 and 675°C, and presumably at higher temperatures, NaNbO₃ is in the cubic perovskite (*E2*₁) structure.
- We use the data taken by (Sakowski-Cowley, 1969) at room temperature.
- The similar structures are listed in the form ABC₃, where the “A” species are on the (4c) andfirst (4d) sites, the “B” species on the (8e) site, and the “C” species on the second (4d) and the two (8e) sites. The A and B sites are often alloyed.
- If the aflow parameters are set to `--params= a, 1,  $\sqrt{8}$ , 1/4, 3/4, 1/4, 1/4, 1/4, 3/4, 1/4, 3/4, 5/8, 1/2, 1/2, 5/8, 0, 0, 5/8` then the structure is equivalent to cubic perovskite *E2*₁.

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B₁	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(4c)	Na I
B₂	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4c)	Na I
B₃	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}}$	(4c)	Na I
B₄	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4c)	Na I
B₅	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}}$	(4c)	O I
B₆	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4c)	O I
B₇	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}}$	(4c)	O I

$\mathbf{B}_8$	$=$	$x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_9$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Na II
$\mathbf{B}_{10}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Na II
$\mathbf{B}_{11}$	$=$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	Na II
$\mathbf{B}_{12}$	$=$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	Na II
$\mathbf{B}_{13}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{14}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{15}$	$=$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{16}$	$=$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B}_{17}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B}_{18}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B}_{19}$	$=$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B}_{20}$	$=$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B}_{21}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B}_{22}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B}_{23}$	$=$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B}_{24}$	$=$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B}_{25}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B}_{26}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B}_{27}$	$=$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B}_{28}$	$=$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B}_{29}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B}_{30}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B}_{31}$	$=$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B}_{32}$	$=$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B}_{33}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8e)	O IV
$\mathbf{B}_{34}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O IV
$\mathbf{B}_{35}$	$=$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O IV
$\mathbf{B}_{36}$	$=$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8e)	O IV
$\mathbf{B}_{37}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8e)	O IV
$\mathbf{B}_{38}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O IV
$\mathbf{B}_{39}$	$=$	$x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	O IV
$\mathbf{B}_{40}$	$=$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8e)	O IV

References

- [1] A. C. Sakowski-Cowley, K. Lukaszewicz, and H. D. Megaw, *The structure of sodium niobate at room temperature, and the problem of reliability in pseudosymmetric structures*, Acta Crystallogr. Sect. B **25**, 851–865 (1969), doi:10.1107/S0567740869003141.

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

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.