# Lueshite (NaNbO₃) Structure: ABC3_oP40_57_cd_e_cd2e-001

This structure originally had the label `ABC3_oP40_57_cd_e_cd2e`. Calls to that address will be redirected here.

https://aflow.org/p/1JM3

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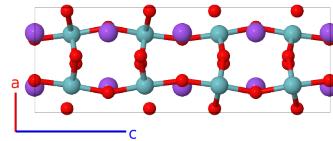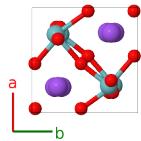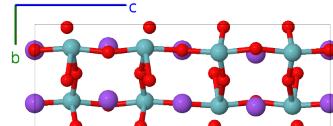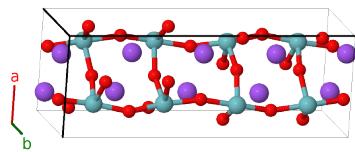
| Prototype	NaNbO₃
AFLOW prototype label	ABC3_oP40_57_cd_e_cd2e-001
Mineral name	lueshite
ICSD	23239
Pearson symbol	oP40
Space group number	57
Space group symbol	$Pbcm$
AFLOW prototype command	`aflow --proto=ABC3_oP40_57_cd_e_cd2e-001` `--params=`$a, b/a, c/a, x_1, x_2, x_3, y_3, x_4, y_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

Other compounds with this structure

NaNb$_{1-x}$Ti$_x$O$_3$

- Another possible structure for NaNbO₃ has been identified.

- 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
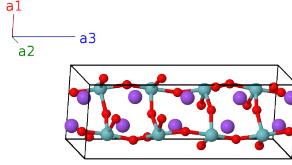
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2}$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4c)	Na I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2}$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}}$	(4c)	Na I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2}$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4c)	O I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \frac{1}{2}\,\mathbf{a_3}$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2}$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}}$	(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
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Na II
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$ax_3\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} + \frac{1}{4}\,\mathbf{a_3}$	=	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	O II
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} + \frac{3}{4}\,\mathbf{a_3}$	=	$ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} - z_5\,\mathbf{a_3}$	=	$ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{22}}$	=	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B_{23}}$	=	$x_5\,\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	=	$ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Nb I
$\mathbf{B_{24}}$	=	$-x_5\,\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{26}}$	=	$-x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B_{27}}$	=	$-x_6\,\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B_{28}}$	=	$x_6\,\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} - z_6\,\mathbf{a_3}$	=	$ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{30}}$	=	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	O III
$\mathbf{B_{31}}$	=	$x_6\,\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	=	$ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	O III

$$\mathbf{B_{32}} = -x_6\,\mathbf{a}_1 + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a}_2 + z_6\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \qquad (8e) \qquad \text{O III}$$

$$\mathbf{B_{33}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (8e) \qquad \text{O IV}$$

$$\mathbf{B_{34}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8e) \qquad \text{O IV}$$

$$\mathbf{B_{35}} = -x_7\,\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8e) \qquad \text{O IV}$$

$$\mathbf{B_{36}} = x_7\,\mathbf{a}_1 - \left(y_7 - \tfrac{1}{2}\right)\mathbf{a}_2 - z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (8e) \qquad \text{O IV}$$

$$\mathbf{B_{37}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (8e) \qquad \text{O IV}$$

$$\mathbf{B_{38}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8e) \qquad \text{O IV}$$

$$\mathbf{B_{39}} = x_7\,\mathbf{a}_1 - \left(y_7 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\hat{\mathbf{z}} \qquad (8e) \qquad \text{O IV}$$

$$\mathbf{B_{40}} = -x_7\,\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (8e) \qquad \text{O IV}$$

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.

Found in

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