$NaNbO_3$ *Cmcm* Lueshite Perovskite Structure: ABC3_oC40_63_2c_d_efg-001

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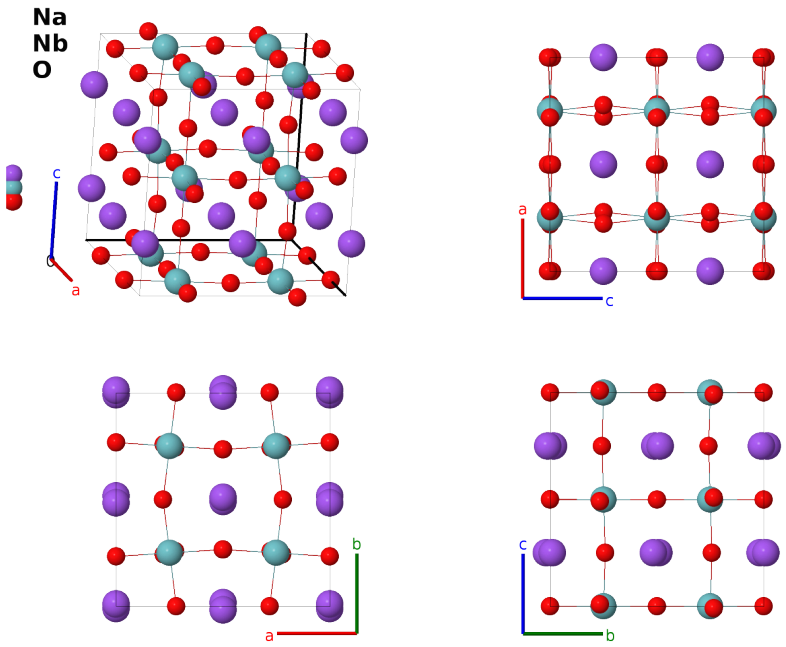
https://aflow.org/prototype-encyclopedia/GWNF

https://aflow.org/prototype-encyclopedia/ABC3_oC40_63_2c_d_efg-001



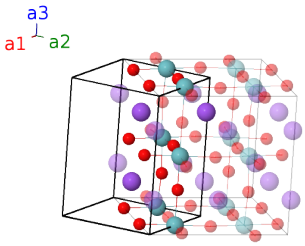
Prototype	$NaNbO_3$
AFLOW prototype label	ABC3_oC40_63_2c_d_efg-001
ICSD	192404
CCDC	1701289
Pearson symbol	oC40
Space group number	63
Space group symbol	*Cmcm*
AFLOW prototype command	`aflow --proto=ABC3_oC40_63_2c_d_efg-001 --params=`$a, b/a, c/a, y_1, y_2, x_4, y_5, z_5, x_6, y_6$

Other compounds with this structure
$AgNbO_3$, $AgTaO_3$, $BrSAg_3$, $NaTaO_3$, $SrHfO_3$, $SrZrO_3$

- 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 (this structure)
  - 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.
- We use the data taken at 575°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 (8d) site, and the "C" species on the (8e), (8f), and (8g) sites. The A and B sites are often alloyed.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(8d)	Nb I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Nb I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}}$	(8d)	Nb I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}}$	(8e)	O I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}$	(8e)	O I
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{13}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{14}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{15}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{16}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8f)	O II

$\mathbf{B_{17}}$	=	$(x_6 - y_6)\ \mathbf{a}_1 + (x_6 + y_6)\ \mathbf{a}_2 + \frac{1}{4}\ \mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{18}}$	=	$-(x_6 - y_6)\ \mathbf{a}_1 - (x_6 + y_6)\ \mathbf{a}_2 + \frac{3}{4}\ \mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{19}}$	=	$-(x_6 + y_6)\ \mathbf{a}_1 - (x_6 - y_6)\ \mathbf{a}_2 + \frac{1}{4}\ \mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	O III
$\mathbf{B_{20}}$	=	$(x_6 + y_6)\ \mathbf{a}_1 + (x_6 - y_6)\ \mathbf{a}_2 + \frac{3}{4}\ \mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	O III

References

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

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