Paraelectric $LiNbO_3$ Structure: ABC3_hR10_167_a_b_e-001

This structure originally had the label `ABC3_hR10_167_a_b_e.LiNbO3`. Calls to that address will be redirected here.

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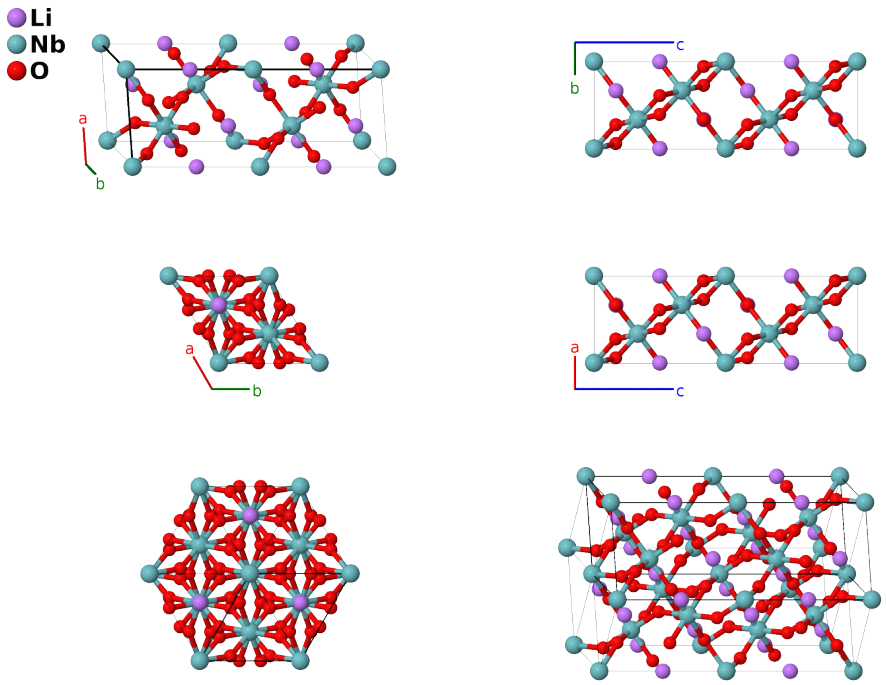
https://aflow.org/p/TXPE

https://aflow.org/p/ABC3_hR10_167_a_b_e-001

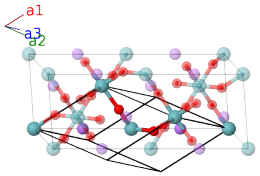


Prototype	$LiONbO_3$
AFLOW prototype label	ABC3_hR10_167_a_b_e-001
ICSD	81240
Pearson symbol	hR10
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=ABC3_hR10_167_a_b_e-001 --params=`$a, c/a, x_3$

- This is the paraelectric phase, stable above 1430K. There is also a ferroelectric phase.
- Paraelectric $LiNbO_3$ and calcite $CaCO_3$ have the same AFLOW prototype label, ABC3_hR10_167_a_b_e. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings rhombohedral structures can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B_3}$	=	0	=	0	(2b)	Nb I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Nb I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_3 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_3 - 1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_7}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_3 + 3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_3 + 1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_9}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_3 - 1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_3 + 5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I
$\mathbf{B_{10}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	O I

References

[1] H. Boysen and F. Altorfer, *A neutron powder investigation of the high-temperature structure and phase transition in $LiNbO_3$*, Acta Crystallogr. Sect. B **50**, 405–414 (1994), doi:10.1107/S0108768193012820.