

Paraelectric LiNbO₃ Structure: ABC3_hR10_167_a_b_e-001

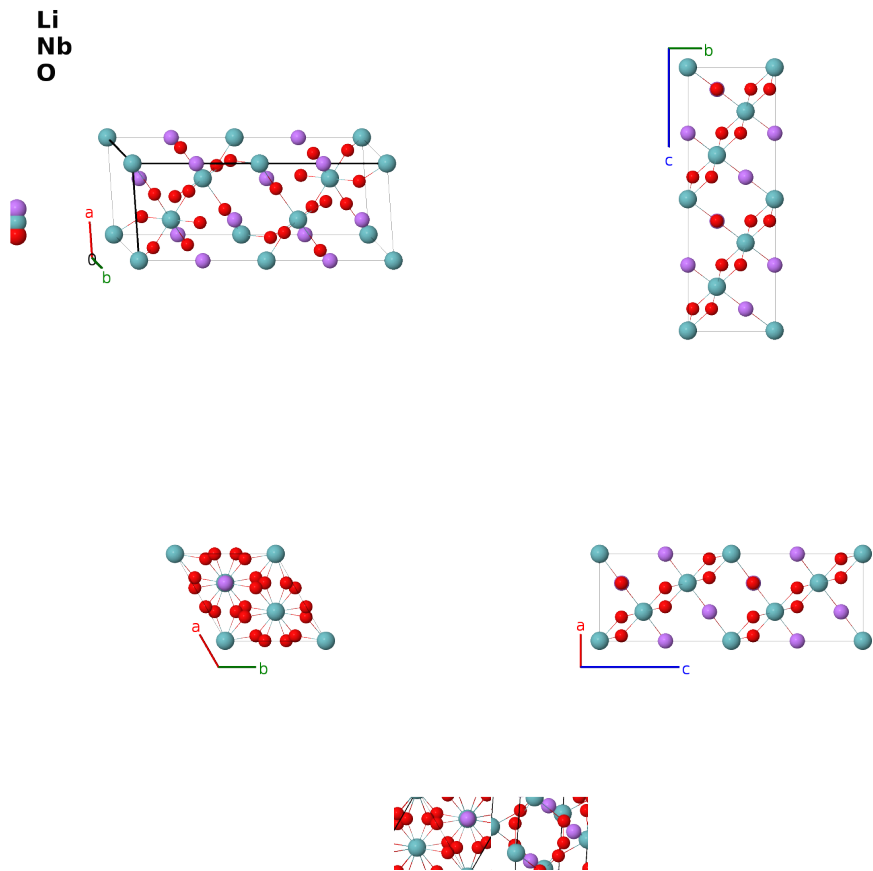
This structure previously used the label(s) **ABC3_hR10_167_a_b_e.LiNbO3**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/TXPE>

https://aflow.org/prototype-encyclopedia/ABC3_hR10_167_a_b_e-001



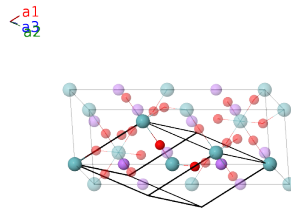
Prototype	LiONbO ₃
AFLOW prototype label	ABC3_hR10_167_a_b_e-001
ICSD	81240
CCDC	1641394
Pearson symbol	hR10
Space group number	167
Space group symbol	$R\bar{3}c$

AFLOW prototype command `aflow --proto=ABC3_hR10_167_a_b_e-001`
 `--params=a,c/a,x3`

- This is the paraelectric phase, stable above 1430K. There is also a ferroelectric phase.
- Paraelectric LiNbO₃ and calcite CaCO₃ 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

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



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
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a (4x_3 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$		(6e)	O I
$\mathbf{B}_6$	$= \frac{1}{4} \mathbf{a}_1 + x_3 \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a (4x_3 - 1) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$		(6e)	O I
$\mathbf{B}_7$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$		(6e)	O I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{8}a (4x_3 + 3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a (12x_3 + 1) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$		(6e)	O I
$\mathbf{B}_9$	$= \frac{3}{4} \mathbf{a}_1 - x_3 \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{8}a (4x_3 - 1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a (12x_3 + 5) \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$		(6e)	O I
$\mathbf{B}_{10}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{5}{12}c \hat{\mathbf{z}}$		(6e)	O I

References

- [1] H. Boysen and F. Altorfer, *A neutron powder investigation of the high-temperature structure and phase transition in LiNbO₃*, Acta Crystallogr. Sect. B **50**, 405–414 (1994), doi:10.1107/S0108768193012820.

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