

Ferroelectric LiNbO₃ Structure: ABC3_hR10_161_a_a_b-001

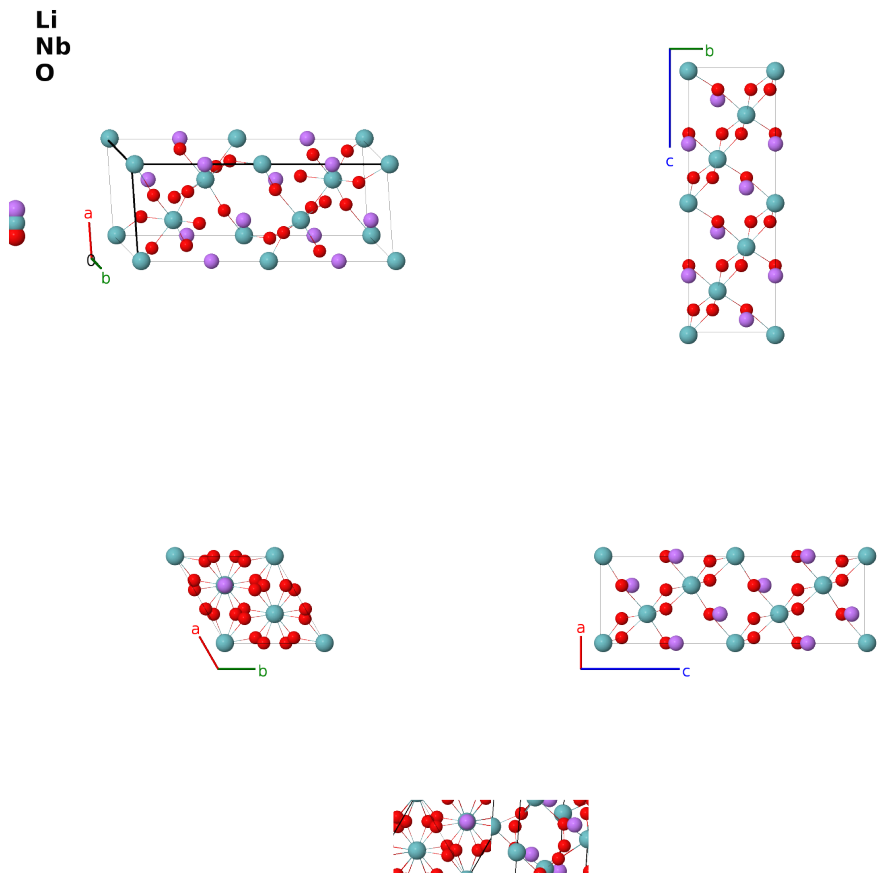
This structure previously used the label(s) **ABC3_hR10_161_a_a_b**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/FZF0>

https://aflow.org/prototype-encyclopedia/ABC3_hR10_161_a_a_b-001



Prototype	LiNbO ₃
AFLOW prototype label	ABC3_hR10_161_a_a_b-001
ICSD	81243
CCDC	1641396
Pearson symbol	hR10
Space group number	161
Space group symbol	<i>R</i> 3 <i>c</i>

AFLOW prototype command `aflow --proto=ABC3_hR10_161_a_a_b-001`
 `--params=a, c/a, x1, x2, x3, y3, z3`

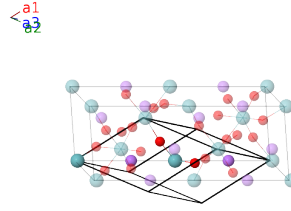
Other compounds with this structure

BiFeO₃, CsPbF₃

- This is the ferroelectric phase of LiNbO₃, which is stable below 1430K. There is also a high-temperature paraelectric phase.
- In the special case $c/a = \sqrt{6}$, $z_1 = 1/4$, $z_2 = 0$, $x_3 = 1/2$, $y_3 = 0$, $z_3 = 0$ this reduces to a double unit cell version of the cubic perovskite ($E2_1$) structure. This sets the angle between the rhombohedral primitive vectors to 60°. Experimentally the value is about 56°.

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B}_2$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Li I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B}_4$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(2a)	Nb I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B}_6$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B}_7$	$= y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B}_8$	$= \left(z_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{6}c(2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B}_9$	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{6}c(2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B}_{10}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{6}c(2x_3 + 2y_3 + 2z_3 + 3) \hat{\mathbf{z}}$	(6b)	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.

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