Ferroelectric $LiNbO_3$ Structure: ABC3_hR10_161_a_a_b-001

This structure originally had the label `ABC3_hR10_161_a_a_b`. Calls to that address will be redirected here.

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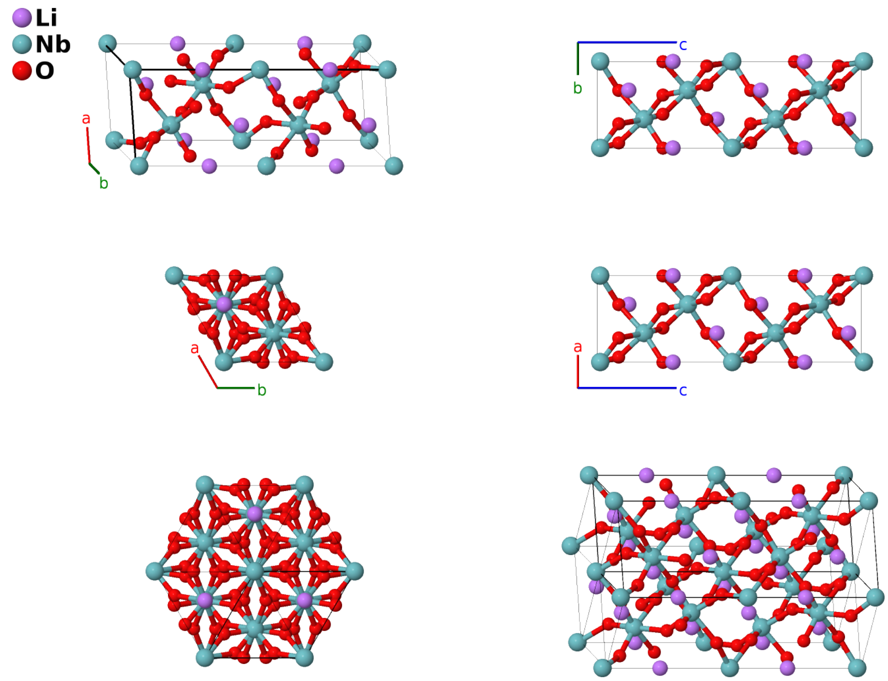
https://aflow.org/p/FZF0

https://aflow.org/p/ABC3_hR10_161_a_a_b-001



Prototype	$LiNbO_3$
AFLOW prototype label	ABC3_hR10_161_a_a_b-001
ICSD	81243
Pearson symbol	hR10
Space group number	161
Space group symbol	$R3c$
AFLOW prototype command	`aflow --proto=ABC3_hR10_161_a_a_b-001` `--params=`$a, c/a, x_1, x_2, x_3, y_3, z_3$

Other compounds with this structure

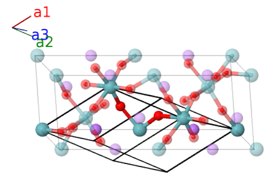
$BiFeO_3$, $CsPbF_3$

- This is the ferroelectric phase of $LiNbO_3$, 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

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(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
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3 - z_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3 - 2y_3 + z_3\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B_6}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(y_3 - z_3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_3 - y_3 - z_3\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B_7}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3 - y_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3 + y_3 - 2z_3\right)\hat{\mathbf{y}} + \frac{1}{3}c\left(x_3 + y_3 + z_3\right)\hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B_8}$	=	$\left(z_3 + \frac{1}{2}\right)\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3 - z_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3 - 2y_3 + z_3\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_3 + 2y_3 + 2z_3 + 3\right)\hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B_9}$	=	$\left(y_3 + \frac{1}{2}\right)\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\left(y_3 - z_3\right)\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\left(2x_3 - y_3 - z_3\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_3 + 2y_3 + 2z_3 + 3\right)\hat{\mathbf{z}}$	(6b)	O I
$\mathbf{B_{10}}$	=	$\left(x_3 + \frac{1}{2}\right)\mathbf{a}_1 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3 - y_3\right)\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\left(x_3 + y_3 - 2z_3\right)\hat{\mathbf{y}} + \frac{1}{6}c\left(2x_3 + 2y_3 + 2z_3 + 3\right)\hat{\mathbf{z}}$	(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.