γ-$LiAlO_2$ Structure: ABC2_tP16_92_a_a_b-001

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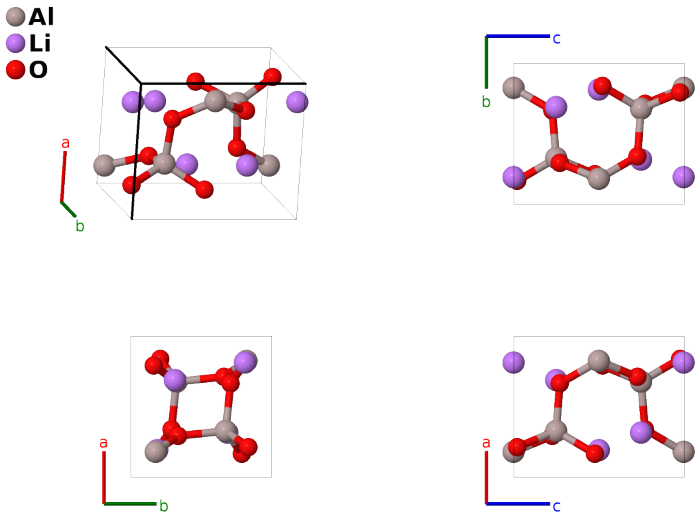


Prototype	$AlLiO_2$
AFLOW prototype label	ABC2_tP16_92_a_a_b-001
ICSD	23815
Pearson symbol	tP16
Space group number	92
Space group symbol	$P4_12_12$
AFLOW prototype command	`aflow --proto=ABC2_tP16_92_a_a_b-001 --params=`$a, c/a, x_1, x_2, x_3, y_3, z_3$

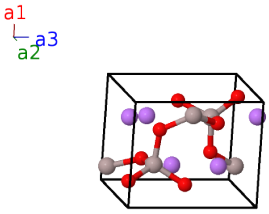
Other compounds with this structure
$NaAlO_2$, $NaFeO_2$

- $LiAlO_2$ exists in many different forms. We describe them using the notation of (Liu, 2018):
  - α, synthesized from Al_2O_3 and Li_2CO_3 at 600°C (Marezio, 1966) forms in the Caswellsilverite $F5_1$ structure, space group $R\bar{3}m$ #166.
  - β is the low temperature structure (Thery, 1961) forming in the $LiGaO_2$ structure, space group $Pna2_1$ #33.
  - β' is a high-pressure monoclinic phase formed at 1.8 GPa and 370°C, but there is not enough information provided to determine either the space group or occupied Wyckoff positions (Chang, 1968).
  - γ (this structure) is the standard phase under ambient conditions. It is tetragonal (Marezio, 1965), space group $P4_12_12$ #92.

  - δ is formed at high pressures (9 GPa) under shock compression and takes the γ-$LiFeO_2$ structure.
  - ϵ, formed from Al_2O_3 and LiH at 500°C, (Debray, 1960) is a cubic phase (space group $I4_132$ #214) with 48 formula units in a cube 12.65Å on a side, but the atomic positions were not determined.
  - ζ is a predicted high-pressure monoclinic structure (Liu, 2018), (space group $C2/m$ #12). It is apparently not related to the β' phase.
- The α, β' and δ phases are metastable under ambient conditions, but transform to γ-$LiAlO_2$ upon heating. (Liu, 2008)

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}}$	(4a)	Al I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_3}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(4a)	Li I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Li I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{11}}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{12}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{13}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{14}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{15}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B_{16}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O I

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