Predicted ζ-$LiAlO_2$ Structure: ABC2_mC24_12_ah_cg_ij-001

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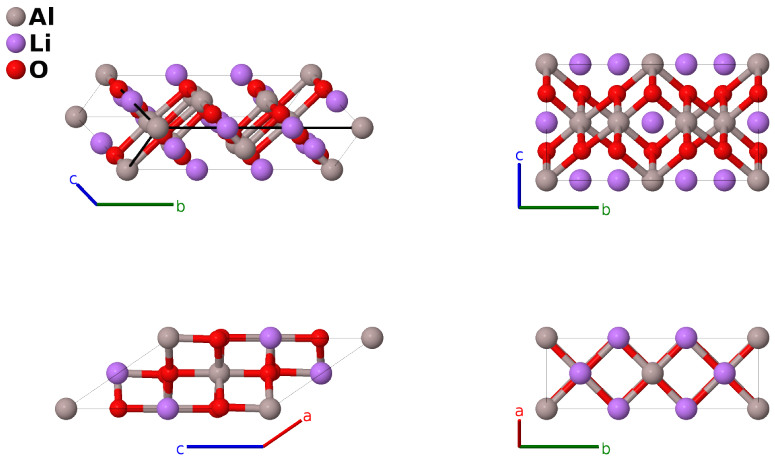
https://aflow.org/p/JWKX

https://aflow.org/p/ABC2_mC24_12_ah_cg_ij-001



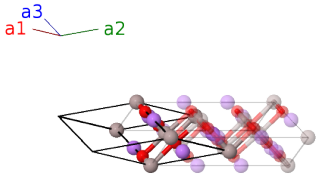
Prototype	$AlLiO_2$
AFLOW prototype label	ABC2_mC24_12_ah_cg_ij-001
ICSD	none
Pearson symbol	mC24
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=ABC2_mC24_12_ah_cg_ij-001 --params=`$a, b/a, c/a, \beta, y_3, y_4, x_5, z_5, x_6, y_6, z_6$

- $LiAlO_2$ 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 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 (this structure) 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)
- Data for ζ-$LiAlO_2$ was taken from the calculations of (Liu, 2018) at 40 GPa.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2c)	Li I
$\mathbf{B_3}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$by_3\,\hat{\mathbf{y}}$	(4g)	Li II
$\mathbf{B_4}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-by_3\,\hat{\mathbf{y}}$	(4g)	Li II
$\mathbf{B_5}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	Al II
$\mathbf{B_6}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	Al II
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_9}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B_{10}}$	=	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B_{11}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B_{12}}$	=	$(x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II

References

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