γ-$LiAlO_2$ Structure: ABC2_tP16_92_a_a_b-001

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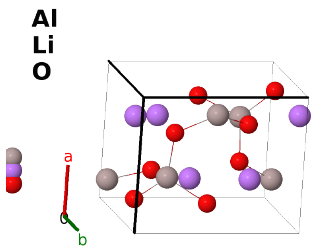
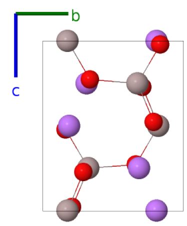
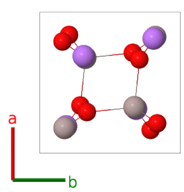
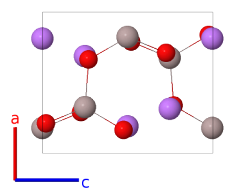
https://aflow.org/prototype-encyclopedia/ABC2_tP16_92_a_a_b-001









Prototype	$AlLiO_2$
AFLOW prototype label	ABC2_tP16_92_a_a_b-001
ICSD	23815
CCDC	1599890
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

$NaAlO_2$, $NaFeO_2$

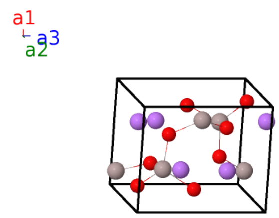
- $LiAlO_2$ exists in many different forms. We describe them using the notation of (Liu, 2018):
  - α, synthesized from Al_2O_3 and Li_2CO_3 at 600°C (Marezio, 1966) forms in the Caswellsilverite $F5_1$ structure, space group $R\bar{3}m$ #166.

- 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)
- Space group $P4_12_12$ #92 is a Sohncke Class II space group, so this structure can also appear in its enantiomorphic twin, $P4_32_12$ #96.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}}$	(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

$\mathbf{B_{14}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_3-\frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\mathbf{\hat{x}}-a\left(y_3-\frac{1}{2}\right)\,\mathbf{\hat{y}}-c\left(z_3-\frac{3}{4}\right)\,\mathbf{\hat{z}}$	(8b)	O I
$\mathbf{B_{15}}$	=	$y_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$ay_3\,\mathbf{\hat{x}}+ax_3\,\mathbf{\hat{y}}-cz_3\,\mathbf{\hat{z}}$	(8b)	O I
$\mathbf{B_{16}}$	=	$-y_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\mathbf{\hat{x}}-ax_3\,\mathbf{\hat{y}}-c\left(z_3-\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O I

References

[1] M. Marezio, *The crystal structure and anomalous dispersion of γ-LiAlO$_2$*, Acta Cryst. **19**, 396–400 (1965), doi:10.1107/S0365110X65003511.

[2] L. Lei, D. He, Y. Zou, W. Zhang, Z. Wang, M. Jiang, and M. Du, *J. Solid State Chem.*, Phase transitions of $LiAlO_2$ at high pressure and high temperature **181**, 1810–1815 (2008), doi:10.1016/j.jssc.2008.04.006.

[3] J. Théry, A.-M. Lejus, D. Briançon, and R. Collongues, *Sur la structure et les propriétés des aluminates alcalins*, Bull. Soc. chim. Fr. pp. 973–975 (1961).

[4] L. Debray and A. Hardy, *Contribution à l'étude structurale des aluminates de lithium*, C. R. Hebd. Séances Acad. Sci. **251**, 725–726 (1960).

Found in

[1] L. Liu and H. Liu, *First principles study of LiAlO$_2$: new dense monoclinic phase under high pressure*, J. Phys.: Condens. Matter **30**, 115401 (2018), doi:10.1088/1361-648X/aaad23.

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