La_3Al_{11} Structure: A11B3_oI28_71_bf2m_ai-001

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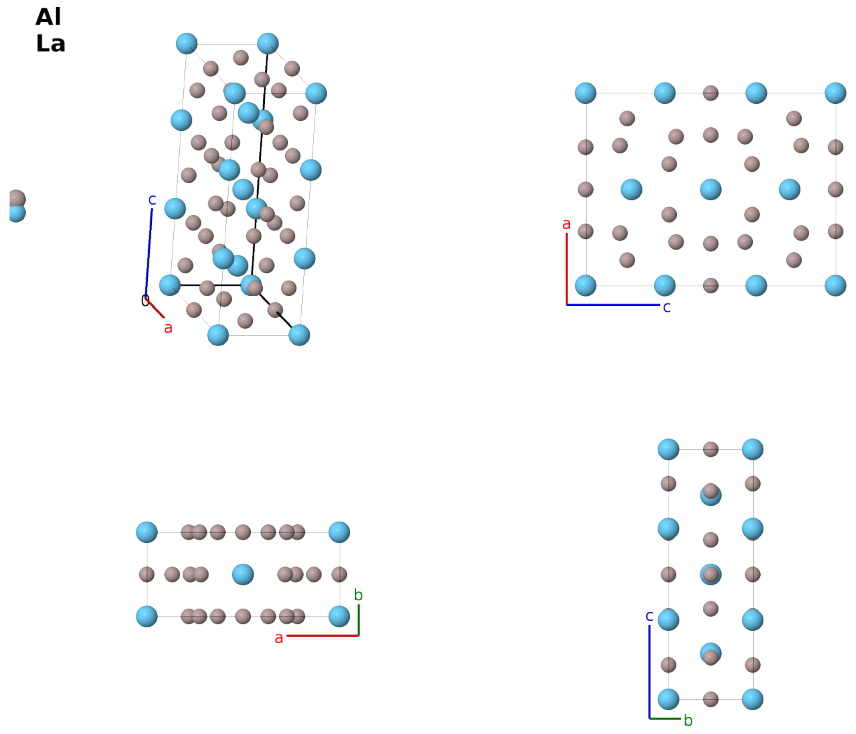
https://aflow.org/prototype-encyclopedia/TNYL

https://aflow.org/prototype-encyclopedia/A11B3_oI28_71_bf2m_ai-001



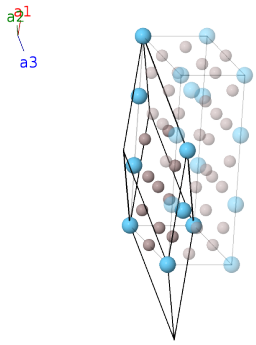
Prototype	$Al_{11}La_3$
AFLOW prototype label	A11B3_oI28_71_bf2m_ai-001
ICSD	57937
CCDC	1621976
Pearson symbol	oI28
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=A11B3_oI28_71_bf2m_ai-001 --params=`$a, b/a, c/a, x_3, z_4, x_5, z_5, x_6, z_6$

Other compounds with this structure

Ce_3Al_{11}, $(La_{\frac{1}{2}}Nd_{\frac{1}{2}})_3Al_{11}$, Sr_3In_{11}, Yb_3Zn_{11}, $Yb_3(Al_xZn_{11-x}$, $Ce_3(Al_{9.13}Ga_{1.78}Ni_{0.08})$

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	La I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Al I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	Al II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$	(4f)	Al II
$\mathbf{B_5}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4i)	La II
$\mathbf{B_6}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4i)	La II
$\mathbf{B_7}$	=	$z_5\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(8m)	Al III
$\mathbf{B_8}$	=	$z_5\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(8m)	Al III
$\mathbf{B_9}$	=	$-z_5\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(8m)	Al III
$\mathbf{B_{10}}$	=	$-z_5\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(8m)	Al III
$\mathbf{B_{11}}$	=	$z_6\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(8m)	Al IV
$\mathbf{B_{12}}$	=	$z_6\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(8m)	Al IV
$\mathbf{B_{13}}$	=	$-z_6\,\mathbf{a}_1 - (x_6 + z_6)\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$	(8m)	Al IV
$\mathbf{B_{14}}$	=	$-z_6\,\mathbf{a}_1 + (x_6 - z_6)\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$	(8m)	Al IV

References

[1] A. H. G. de Mesquita and K. H. J. Buschow, *The crystal structure of so-called α-$LaAl_4$ (La_3Al_{11})*, Acta Cryst. **22**, 497–501 (1967), doi:10.1107/S0365110X67001045.

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[1] O. Janka, T. Shang, R. E. Baumbach, E. D. Bauer, J. D. Thompson, and S. M. Kauzlarich, *Structure and Magnetic Properties of $Ce_3(Ni/Al/Ga)_{11}$-A New Phase with the La_3Al_{11} Structure Type*, Crystals **5**, 1–8 (2015), doi:10.3390/cryst5010001.

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