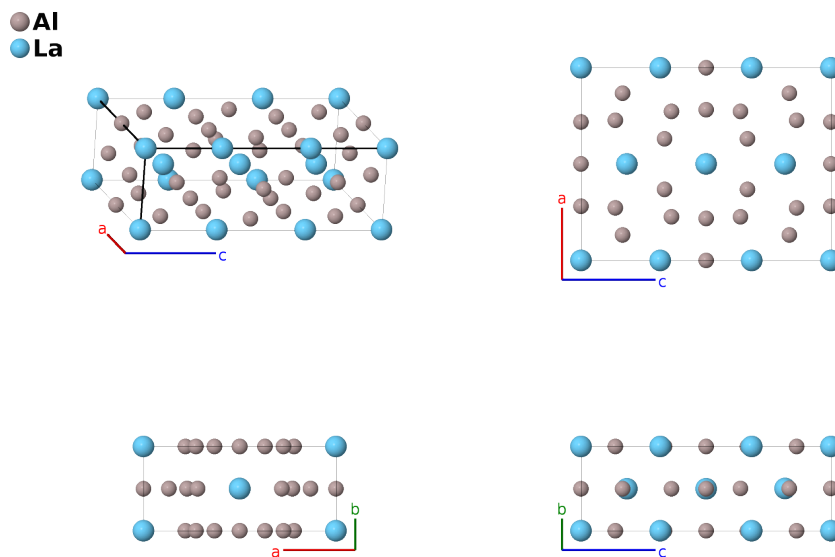


La₃Al₁₁ Structure: A11B3_oI28_71_bf2m_ai-001

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<https://aflow.org/p/TNYL>

https://aflow.org/p/A11B3_oI28_71_bf2m_ai-001

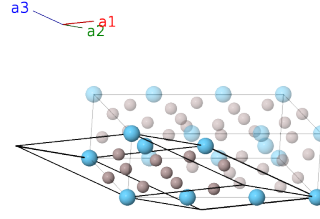


Prototype	Al ₁₁ La ₃
AFLOW prototype label	A11B3_oI28_71_bf2m_ai-001
ICSD	57937
Pearson symbol	oI28
Space group number	71
Space group symbol	<i>Immm</i>
AFLOW prototype command	aflow --proto=A11B3_oI28_71_bf2m_ai-001 --params=a, b/a, c/a, x ₃ , z ₄ , x ₅ , z ₅ , x ₆ , z ₆

Other compounds with this structure

Ce₃Al₁₁, (La_{1/2}Nd_{1/2})₃Al₁₁, Sr₃In₁₁, Yb₃Zn₁₁, Yb₃(Al_xZn_{11-x}), Ce₃(Al_{0.13}Ga_{1.78}Ni_{0.08})

Body-centered Orthorhombic primitive vectors



$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}} - \frac{1}{2}c\hat{\mathbf{z}}\end{aligned}$$

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	$\frac{1}{2}\mathbf{a}_1 + x_3\mathbf{a}_2 + (x_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}}$	(4f)	Al II
\mathbf{B}_4	$\frac{1}{2}\mathbf{a}_1 - x_3\mathbf{a}_2 - (x_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}}$	(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

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