

AlLi₃N₂ (*E9_d*) Structure: AB3C2_cI96_206_c_e_ad-001

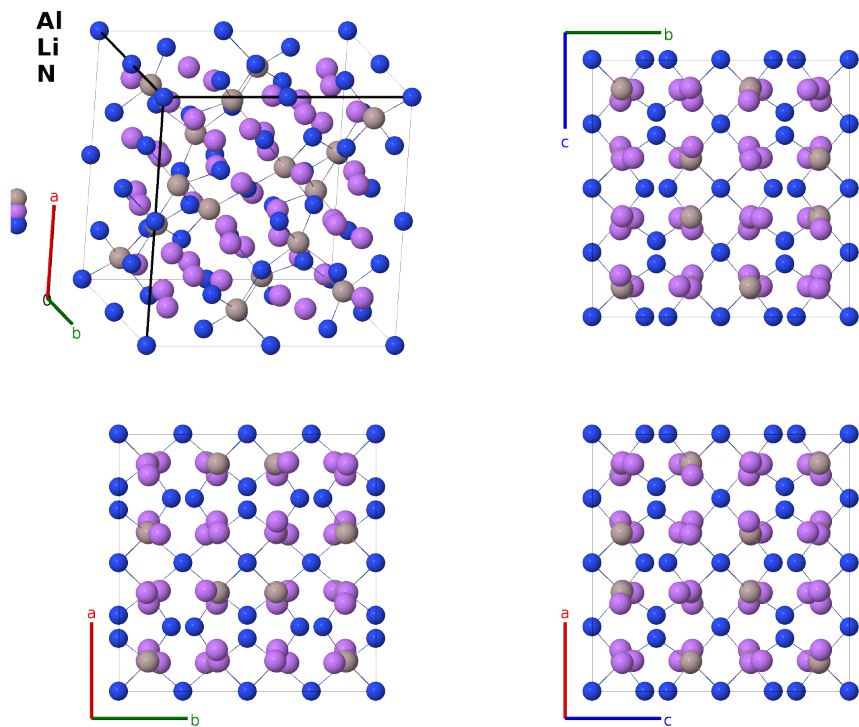
This structure previously used the label(s) **AB3C2_cI96_206_c_e_ad**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/WEUP>

https://aflow.org/prototype-encyclopedia/AB3C2_cI96_206_c_e_ad-001



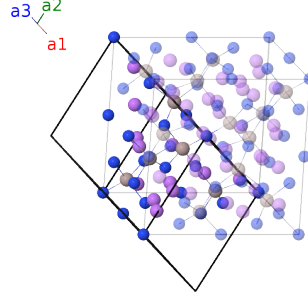
Prototype	AlLi ₃ N ₂
AFLOW prototype label	AB3C2_cI96_206_c_e_ad-001
<i>Strukturbericht</i> designation	<i>E9_d</i>
ICSD	25565
CCDC	1601219
Pearson symbol	cI96
Space group number	206
Space group symbol	<i>Ia</i> $\bar{3}$
AFLOW prototype command	<code>aflow --proto=AB3C2_cI96_206_c_e_ad-001</code> <code>--params=<i>a</i>, <i>x</i>₂, <i>x</i>₃, <i>x</i>₄, <i>y</i>₄, <i>z</i>₄</code>

Other compounds with this structure

GaLi₃N₂, ScLi₃N₂, TiLi₃N₂, ZnLi₃N₂, SiLi₃N₂, GeLi₃N₂

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(8a)	N I
$\mathbf{B}_2$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{y}}$	(8a)	N I
$\mathbf{B}_3$	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}}$	(8a)	N I
$\mathbf{B}_4$	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{2}a\hat{\mathbf{z}}$	(8a)	N I
$\mathbf{B}_5$	$2x_2\mathbf{a}_1 + 2x_2\mathbf{a}_2 + 2x_2\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_6$	$\frac{1}{2}\mathbf{a}_1 - (2x_2 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} - a(x_2 - \frac{1}{2})\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_7$	$-(2x_2 - \frac{1}{2})\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2})\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_8$	$-(2x_2 - \frac{1}{2})\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$ax_2\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} - a(x_2 - \frac{1}{2})\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_9$	$-2x_2\mathbf{a}_1 - 2x_2\mathbf{a}_2 - 2x_2\mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_{10}$	$\frac{1}{2}\mathbf{a}_1 + (2x_2 + \frac{1}{2})\mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + a(x_2 + \frac{1}{2})\hat{\mathbf{y}} - ax_2\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_{11}$	$(2x_2 + \frac{1}{2})\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2})\hat{\mathbf{x}} - ax_2\hat{\mathbf{y}} + ax_2\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_{12}$	$(2x_2 + \frac{1}{2})\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$-ax_2\hat{\mathbf{x}} + ax_2\hat{\mathbf{y}} + a(x_2 + \frac{1}{2})\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_{13}$	$\frac{1}{4}\mathbf{a}_1 + (x_3 + \frac{1}{4})\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d)	N II
$\mathbf{B}_{14}$	$\frac{3}{4}\mathbf{a}_1 - (x_3 - \frac{1}{4})\mathbf{a}_2 - (x_3 - \frac{1}{2})\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d)	N II
$\mathbf{B}_{15}$	$x_3\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + (x_3 + \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + ax_3\hat{\mathbf{y}}$	(24d)	N II
$\mathbf{B}_{16}$	$-(x_3 - \frac{1}{2})\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - (x_3 - \frac{1}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	N II
$\mathbf{B}_{17}$	$(x_3 + \frac{1}{4})\mathbf{a}_1 + x_3\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + ax_3\hat{\mathbf{z}}$	(24d)	N II
$\mathbf{B}_{18}$	$-(x_3 - \frac{1}{4})\mathbf{a}_1 - (x_3 - \frac{1}{2})\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(24d)	N II
$\mathbf{B}_{19}$	$\frac{3}{4}\mathbf{a}_1 - (x_3 - \frac{3}{4})\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{z}}$	(24d)	N II
$\mathbf{B}_{20}$	$\frac{1}{4}\mathbf{a}_1 + (x_3 + \frac{3}{4})\mathbf{a}_2 + (x_3 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2})\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d)	N II
$\mathbf{B}_{21}$	$-x_3\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 - (x_3 - \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} - ax_3\hat{\mathbf{y}}$	(24d)	N II
$\mathbf{B}_{22}$	$(x_3 + \frac{1}{2})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + (x_3 + \frac{3}{4})\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + a(x_3 + \frac{1}{2})\hat{\mathbf{y}}$	(24d)	N II
$\mathbf{B}_{23}$	$-(x_3 - \frac{3}{4})\mathbf{a}_1 - x_3\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{y}} - ax_3\hat{\mathbf{z}}$	(24d)	N II
$\mathbf{B}_{24}$	$(x_3 + \frac{3}{4})\mathbf{a}_1 + (x_3 + \frac{1}{2})\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + a(x_3 + \frac{1}{2})\hat{\mathbf{z}}$	(24d)	N II

$$\begin{aligned}
\mathbf{B}_{25} &= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3 = ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{26} &= (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{27} &= (y_4 - z_4) \mathbf{a}_1 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 = -a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{28} &= -(y_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 = ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{29} &= (x_4 + y_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + (x_4 + z_4) \mathbf{a}_3 = az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{30} &= -(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_1 + (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - z_4) \mathbf{a}_3 = az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{31} &= (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 = -az_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{32} &= (x_4 - y_4) \mathbf{a}_1 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 = -a(z_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{33} &= (x_4 + z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3 = ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{34} &= -(x_4 - z_4) \mathbf{a}_1 - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_2 + (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 = -a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{35} &= -(x_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 + (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3 = ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{36} &= (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_3 = -ay_4 \hat{\mathbf{x}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{37} &= -(y_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{38} &= (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 = ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{39} &= -(y_4 - z_4) \mathbf{a}_1 + (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 = a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{40} &= (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 = -ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{41} &= -(x_4 + y_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - (x_4 + z_4) \mathbf{a}_3 = -az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{42} &= (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - z_4) \mathbf{a}_3 = -az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{43} &= (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - z_4) \mathbf{a}_2 + (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 = az_4 \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{44} &= -(x_4 - y_4) \mathbf{a}_1 + (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 = a(z_4 + \frac{1}{2}) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{45} &= -(x_4 + z_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - (y_4 + z_4) \mathbf{a}_3 = -ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (48e) & \text{Li I} \\
\mathbf{B}_{46} &= (x_4 - z_4) \mathbf{a}_1 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 = a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (48e) & \text{Li I}
\end{aligned}$$

$$\mathbf{B}_{47} = \begin{pmatrix} (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = -ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}} \quad (48e) \quad \text{Li I}$$

$$\mathbf{B}_{48} = \begin{pmatrix} (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 - y_4) \mathbf{a}_2 + (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ay_4 \hat{\mathbf{x}} + a(z_4 + \frac{1}{2}) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} \quad (48e) \quad \text{Li I}$$

References

- [1] R. Juza and F. Hund, *Die ternären Nitride Li_3AlN_2 und Li_3GaN_2 . 17. Mitteilung über Metallamide und Metallnitride*, Z. Anorganische und Allgemeine Chemie **257**, 13–25 (1948), doi:10.1002/zaac.19482570102.

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- [1] J. F. Herbst and J. L. G. Hector, *Exploration of the formation of XLi_3N_2 compounds ($X=Sc-Zn$) by means of density functional theory*, Phys. Rev. B **85**, 195137 (2012), doi:10.1103/PhysRevB.85.195137.

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