

Li₇Ge₂ Structure:

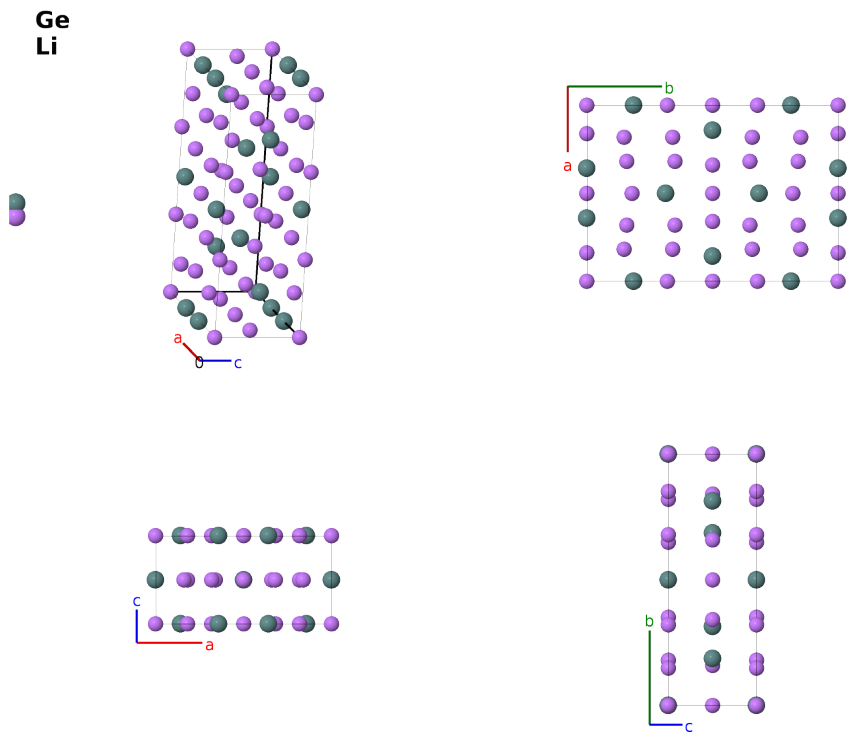
A2B7_oC36_65_gj_achipq-001

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<https://aflow.org/prototype-encyclopedia/3WXX>

https://aflow.org/prototype-encyclopedia/A2B7_oC36_65_gj_achipq-001



Prototype	Ge ₂ Li ₇
AFLOW prototype label	A2B7_oC36_65_gj_achipq-001
ICSD	42063
CCDC	1611774
Pearson symbol	oC36
Space group number	65
Space group symbol	<i>Cmmm</i>
AFLOW prototype command	<code>aflow --proto=A2B7_oC36_65_gj_achipq-001</code> <code>--params=a,b/a,c/a,x₃,x₄,y₅,y₆,x₇,y₇,x₈,y₈</code>

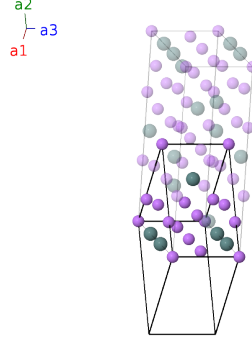
Other compounds with this structure

Li₇Sn₂

- We have shifted the origin by $1/2 (\mathbf{a}_1 + \mathbf{a}_2)$ from that used by (Hopf, 1972).

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	$(2a)$ Li I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	$(2c)$ Li II
$\mathbf{B}_3$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}}$	$(4g)$ Ge I
$\mathbf{B}_4$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}}$	$(4g)$ Ge I
$\mathbf{B}_5$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	$(4h)$ Li III
$\mathbf{B}_6$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	$(4h)$ Li III
$\mathbf{B}_7$	$=$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$by_5 \hat{\mathbf{y}}$	$(4i)$ Li IV
$\mathbf{B}_8$	$=$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-by_5 \hat{\mathbf{y}}$	$(4i)$ Li IV
$\mathbf{B}_9$	$=$	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	$(4j)$ Ge II
$\mathbf{B}_{10}$	$=$	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	$(4j)$ Ge II
$\mathbf{B}_{11}$	$=$	$(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}}$	$(8p)$ Li V
$\mathbf{B}_{12}$	$=$	$-(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}}$	$(8p)$ Li V
$\mathbf{B}_{13}$	$=$	$-(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2$	$=$	$-ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}}$	$(8p)$ Li V
$\mathbf{B}_{14}$	$=$	$(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2$	$=$	$ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}}$	$(8p)$ Li V
$\mathbf{B}_{15}$	$=$	$(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	$(8q)$ Li VI
$\mathbf{B}_{16}$	$=$	$-(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	$(8q)$ Li VI
$\mathbf{B}_{17}$	$=$	$-(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	$(8q)$ Li VI
$\mathbf{B}_{18}$	$=$	$(x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	$(8q)$ Li VI

References

- [1] W. Hopf, W. Müller, and H. Schäfer, *Die Struktur der Phase Li_7Ge_2* , Z. Naturforsch. B **27**, 1157–1160 (1972), doi:10.1515/znbb-1972-1009.

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