Li_7Ge_2 Structure: A2B7_oC36_65_gj_achipq-001

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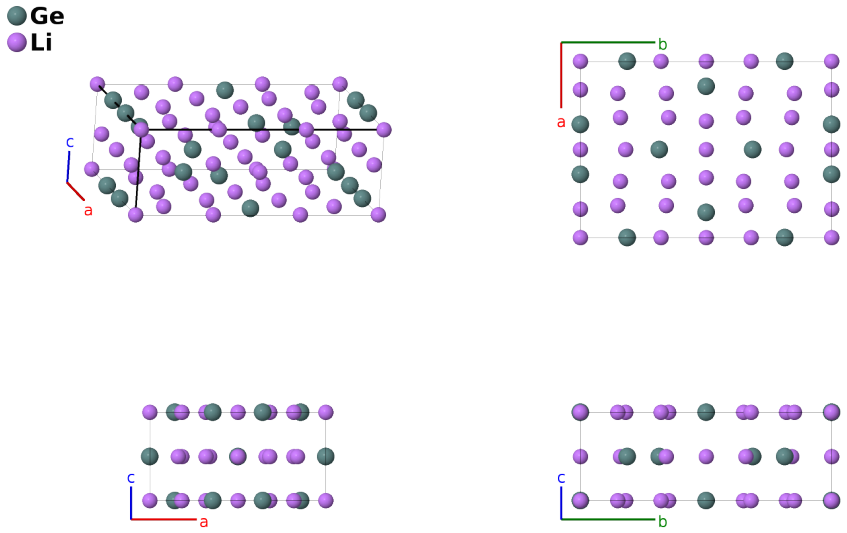
https://aflow.org/p/3WXK

https://aflow.org/p/A2B7_oC36_65_gj_achipq-001



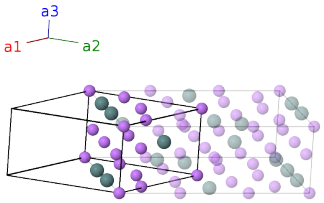
Prototype	Ge_2Li_7
AFLOW prototype label	A2B7_oC36_65_gj_achipq-001
ICSD	42063
Pearson symbol	oC36
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=A2B7_oC36_65_gj_achipq-001 --params=`$a, b/a, c/a, x_3, x_4, y_5, y_6, x_7, y_7, x_8, y_8$

Other compounds with this structure
Li_7Sn_2

- 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

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



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/znb-1972-1009.