

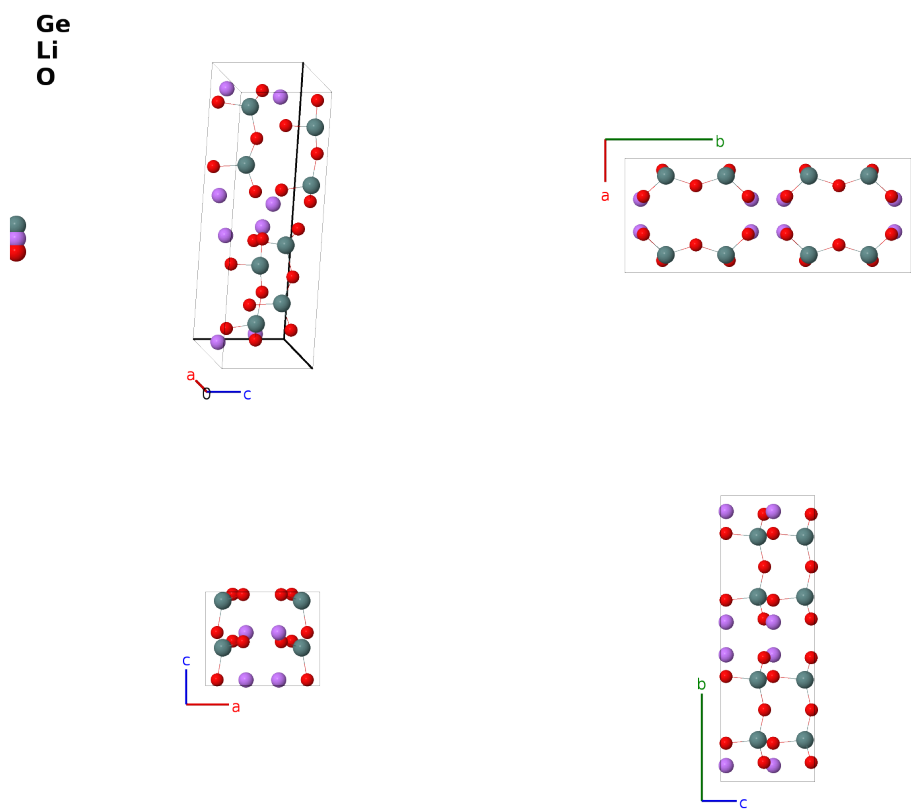
Li₂(Si_{0.25}Ge_{0.75})₂O₅ Structure: A2B2C5_oC36_39_d_d_c2d-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/GBE5>

https://aflow.org/prototype-encyclopedia/A2B2C5_oC36_39_d_d_c2d-001

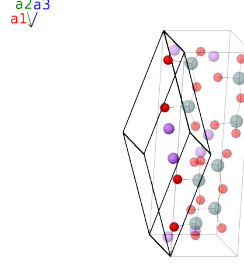


Prototype	Ge ₂ Li ₂ O ₅
AFLOW prototype label	A2B2C5_oC36_39_d_d_c2d-001
ICSD	26836
CCDC	1602215
Pearson symbol	oC36
Space group number	39
Space group symbol	<i>Aem</i> 2
AFLOW prototype command	<code>aflow --proto=A2B2C5_oC36_39_d_d_c2d-001</code> <code>--params=a, b/a, c/a, x₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅</code>

- The germanium (8d) sites are actually 75% germanium and 25% silicon.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 - (z_1 - \frac{1}{4}) \mathbf{a}_2 + (z_1 + \frac{1}{4}) \mathbf{a}_3 =$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - (z_1 - \frac{3}{4}) \mathbf{a}_2 + (z_1 + \frac{3}{4}) \mathbf{a}_3 =$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3 =$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - (y_2 + z_2) \mathbf{a}_2 - (y_2 - z_2) \mathbf{a}_3 =$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 - (y_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 + (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 =$	$ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 + (y_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 + (y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3 =$	$-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8d)	Ge I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3 =$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3 =$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 - (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 =$	$ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 + (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 =$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8d)	Li I
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3 =$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{12}$	$= -x_4 \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3 =$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 - (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 =$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 + (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 =$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B}_{15}$	$= x_5 \mathbf{a}_1 + (y_5 - z_5) \mathbf{a}_2 + (y_5 + z_5) \mathbf{a}_3 =$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{16}$	$= -x_5 \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 - (y_5 - z_5) \mathbf{a}_3 =$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	O III
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 - (y_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 + (-y_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 =$	$ax_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	O III

$$\mathbf{B}_{18} = \begin{matrix} -x_5 \mathbf{a}_1 + (y_5 - z_5 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} \quad (8d) \quad \text{O III}$$

References

- [1] H. Völlenkle, A. Wittmann, and H. Nowotny, *Die Kristallstruktur von $\text{Li}_2(\text{Si}_{0.25}\text{Ge}_{0.75})_2\text{O}_5$* , Z. Kristallogr. **126**, 37–45 (De Kristallstruktur von $\text{Li}_2(\text{Si}_{0.25}\text{Ge}_{0.75})_2\text{O}_5$), doi:10.1524/zkri.1968.126.1-3.37.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).