$LiFe_6Ge_6$ Structure: A6B6C_hP39_191_io_ehjk_ad-001

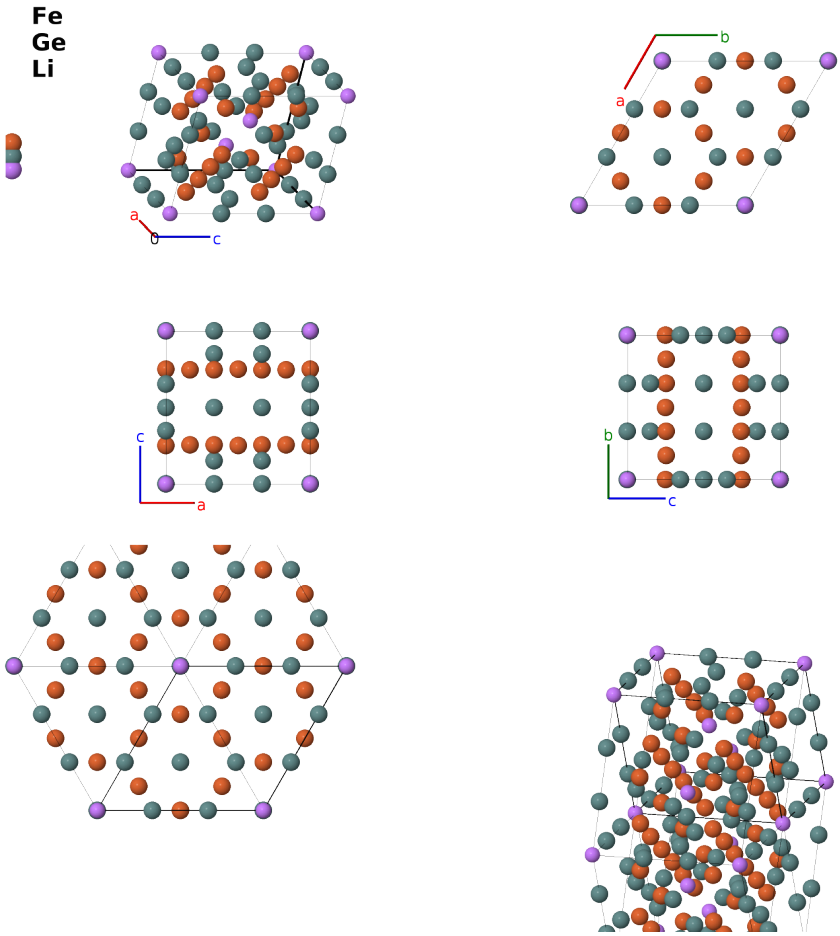
Cite this page as:

- 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/MHVP

https://aflow.org/prototype-encyclopedia/A6B6C_hP39_191_io_ehjk_ad-001



Prototype	Fe_6Ge_6Li
AFLOW prototype label	A6B6C_hP39_191_io_ehjk_ad-001
ICSD	41384
CCDC	1611167
Pearson symbol	hP39
Space group number	191
Space group symbol	$P6/mmm$

AFLOW prototype command `aflow --proto=A6B6C_hP39_191_io_ehjk_ad-001 --params=`$a, c/a, z_3, z_4, z_5, x_6, x_7, x_8, z_8$

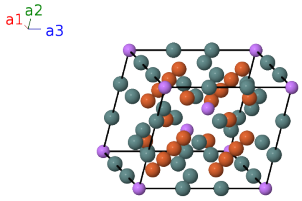
Other compounds with this structure

$LiNi_6Ge_6$, $LiNi_6Si_6$

- All of the $LiFe_xGe_x$ structures are Kagome compounds with the iron, germanium, and lithium/germanium layers all having trihexagonal tiling.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Li I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Li II
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Li II
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2e)	Ge I
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2e)	Ge I
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4h)	Ge II
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4h)	Ge II
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4h)	Ge II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4h)	Ge II
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(6i)	Fe I
$\mathbf{B_{16}}$	=	$x_6\,\mathbf{a}_1$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}$	(6j)	Ge III
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_2$	=	$\frac{1}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}$	(6j)	Ge III
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}}$	(6j)	Ge III
$\mathbf{B_{19}}$	=	$-x_6\,\mathbf{a}_1$	=	$-\frac{1}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}$	(6j)	Ge III
$\mathbf{B_{20}}$	=	$-x_6\,\mathbf{a}_2$	=	$-\frac{1}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}$	(6j)	Ge III
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}}$	(6j)	Ge III
$\mathbf{B_{22}}$	=	$x_7\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_7\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{23}}$	=	$x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_7\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV

$\mathbf{B_{24}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{25}}$	=	$-x_7\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_7\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_7\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{27}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{28}}$	=	$x_8\,\mathbf{a}_1 + 2x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{29}}$	=	$-2x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{30}}$	=	$x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-\sqrt{3}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{31}}$	=	$-x_8\,\mathbf{a}_1 - 2x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_8\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{32}}$	=	$2x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{3}{2}ax_8\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{33}}$	=	$-x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\sqrt{3}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{34}}$	=	$2x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$\frac{3}{2}ax_8\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{35}}$	=	$-x_8\,\mathbf{a}_1 - 2x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_8\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{36}}$	=	$-x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$\sqrt{3}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{37}}$	=	$-2x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{38}}$	=	$x_8\,\mathbf{a}_1 + 2x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$\frac{3}{2}ax_8\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II
$\mathbf{B_{39}}$	=	$x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-\sqrt{3}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12o)	Fe II

References

[1] E. Welk and H.-U. Schuster, *Zur Kenntnis der Phase $LiFe_6Ge_6$*, Z. Anorganische und Allgemeine Chemie **424**, 193–197 (1976), doi:10.1002/zaac.19764240302.

Found in

[1] A. Mantravadi, R. A. Ribeiro, S. L. Bud'ko, P. C. Canfield, and J. V. Zaikina, *Experimental Testing of the Theoretically Predicted Magnetic Properties for Kagomé Compounds in the Li-Fe-Ge System*, Inorg. Chem. **63**, 24697–24708 (2024), doi:10.1021/acs.inorgchem.4c03925.

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).