

# IrGe<sub>4</sub> Structure:

## A4B\_hP15\_144\_4a\_a-001

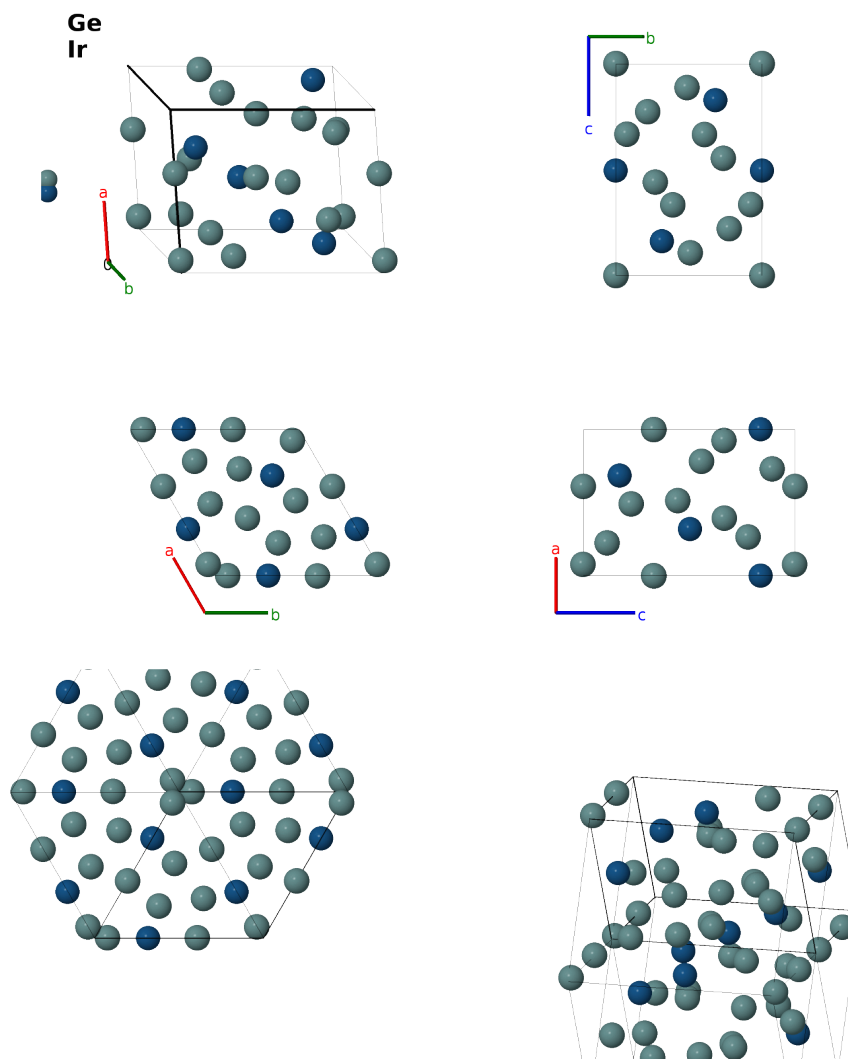
This structure previously used the label(s) **A4B\_hP15\_144\_4a\_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/0VM9>

[https://aflow.org/prototype-encyclopedia/A4B\\_hP15\\_144\\_4a\\_a-001](https://aflow.org/prototype-encyclopedia/A4B_hP15_144_4a_a-001)



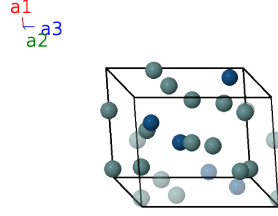
|                       |                       |
|-----------------------|-----------------------|
| Prototype             | Ge <sub>4</sub> Ir    |
| AFLOW prototype label | A4B_hP15_144_4a_a-001 |
| ICSD                  | 197310                |
| CCDC                  | 1924211               |

|                         |                                                                                                                                      |
|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------|
| Pearson symbol          | hP15                                                                                                                                 |
| Space group number      | 144                                                                                                                                  |
| Space group symbol      | $P3_1$                                                                                                                               |
| AFLOW prototype command | aflow --proto=A4B_hP15_144_4a_a-001<br>--params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$ |

- This structure can also be found in the enantiomorphic space group  $P3_2$  # 145.

### Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \hat{\mathbf{z}}
\end{aligned}$$



### Basis vectors

|                   | Lattice coordinates                                                               |   | Cartesian coordinates                                                                                                            | Wyckoff position | Atom type |
|-------------------|-----------------------------------------------------------------------------------|---|----------------------------------------------------------------------------------------------------------------------------------|------------------|-----------|
| $\mathbf{B}_1$    | $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$                          | = | $\frac{1}{2}a(x_1 + y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_1 - y_1) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$             | (3a)             | Ge I      |
| $\mathbf{B}_2$    | $-y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{3}) \mathbf{a}_3$ | = | $\frac{1}{2}a(x_1 - 2y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{3}) \hat{\mathbf{z}}$    | (3a)             | Ge I      |
| $\mathbf{B}_3$    | $-(x_1 - y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + (z_1 + \frac{2}{3}) \mathbf{a}_3$ | = | $-\frac{1}{2}a(2x_1 - y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}} + \frac{1}{3}c(3z_1 + 2) \hat{\mathbf{z}}$ | (3a)             | Ge I      |
| $\mathbf{B}_4$    | $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$                          | = | $\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$             | (3a)             | Ge II     |
| $\mathbf{B}_5$    | $-y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$ | = | $\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{3}) \hat{\mathbf{z}}$    | (3a)             | Ge II     |
| $\mathbf{B}_6$    | $-(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$ | = | $-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{1}{3}c(3z_2 + 2) \hat{\mathbf{z}}$ | (3a)             | Ge II     |
| $\mathbf{B}_7$    | $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$                          | = | $\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$             | (3a)             | Ge III    |
| $\mathbf{B}_8$    | $-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$ | = | $\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$    | (3a)             | Ge III    |
| $\mathbf{B}_9$    | $-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$ | = | $-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$ | (3a)             | Ge III    |
| $\mathbf{B}_{10}$ | $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$                          | = | $\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$             | (3a)             | Ge IV     |
| $\mathbf{B}_{11}$ | $-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$ | = | $\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}}$    | (3a)             | Ge IV     |
| $\mathbf{B}_{12}$ | $-(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$ | = | $-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$ | (3a)             | Ge IV     |
| $\mathbf{B}_{13}$ | $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$                          | = | $\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$             | (3a)             | Ir I      |
| $\mathbf{B}_{14}$ | $-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3$ | = | $\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}}$    | (3a)             | Ir I      |

$$\mathbf{B}_{15} = \begin{matrix} -(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \\ (z_5 + \frac{2}{3}) \mathbf{a}_3 \end{matrix} = \begin{matrix} -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \\ \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}} \end{matrix} \quad (3a) \quad \text{Ir I}$$

## References

- [1] K. Schubert, S. Bhan, T. K. Biswas, K. Frank, and P. K. Panday, *Einige Strukturdaten metallischer Phasen*, Naturwissenschaften **55**, 542–543 (1968), doi:10.1007/BF00660131.

## Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

## First cited in

- D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043