$IrGe_4$ Structure: A4B_hP15_144_4a_a-001

This structure originally had the label `A4B_hP15_144_4a_a`. Calls to that address will be redirected here.

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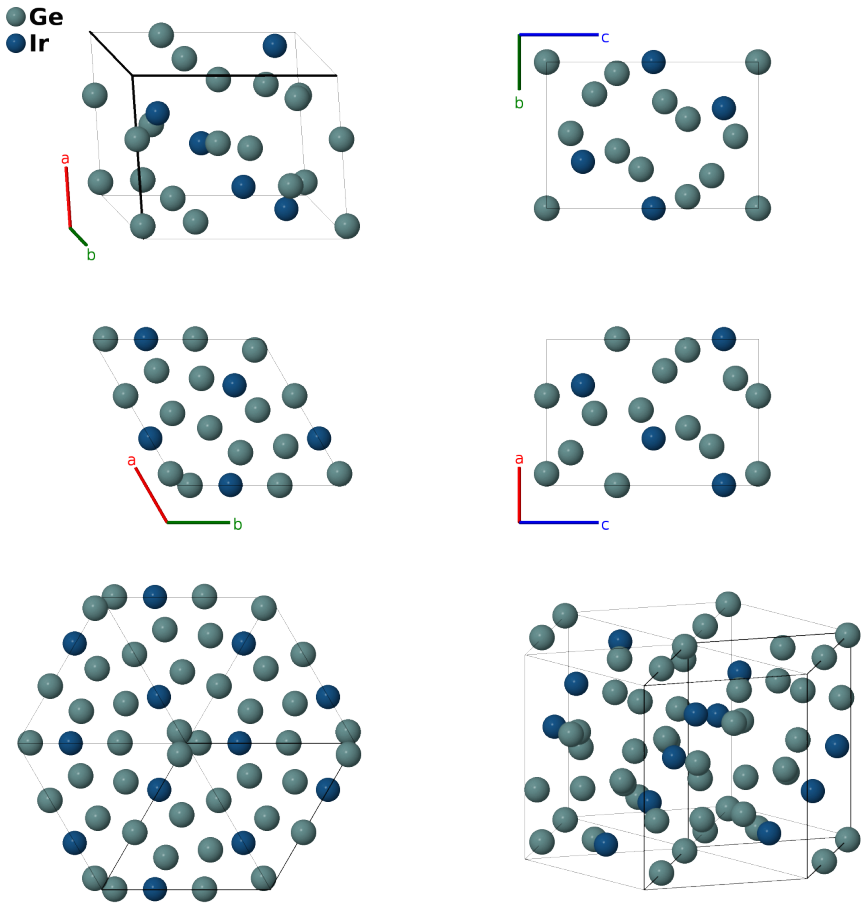
https://aflow.org/p/0VM9

https://aflow.org/p/A4B_hP15_144_4a_a-001

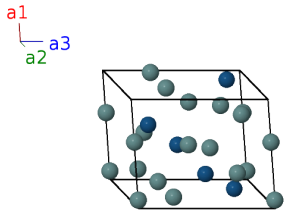


Prototype	Ge_4Ir
AFLOW prototype label	A4B_hP15_144_4a_a-001
ICSD	197310
Pearson symbol	hP15
Space group number	144
Space group symbol	$P3_1$
AFLOW prototype command	`aflow --proto=A4B_hP15_144_4a_a-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

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

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



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
$\mathbf{B_2}$	=	$-y_1\,\mathbf{a}_1 + (x_1 - y_1)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - 2y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(3a)	Ge I
$\mathbf{B_3}$	=	$-(x_1 - y_1)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(z_1 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_1 + 2)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_5}$	=	$-y_2\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(3a)	Ge II
$\mathbf{B_6}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_2 + 2)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_8}$	=	$-y_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(3a)	Ge III
$\mathbf{B_9}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3 + 2)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(3a)	Ge IV
$\mathbf{B_{12}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_4 + 2)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(3a)	Ir I
$\mathbf{B_{15}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_5 + 2)\,\hat{\mathbf{z}}$	(3a)	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.