$Ba_3Ir_4Ge_{16}$ Structure: A3B16C4_tI46_139_ad_2ejm_g2-001

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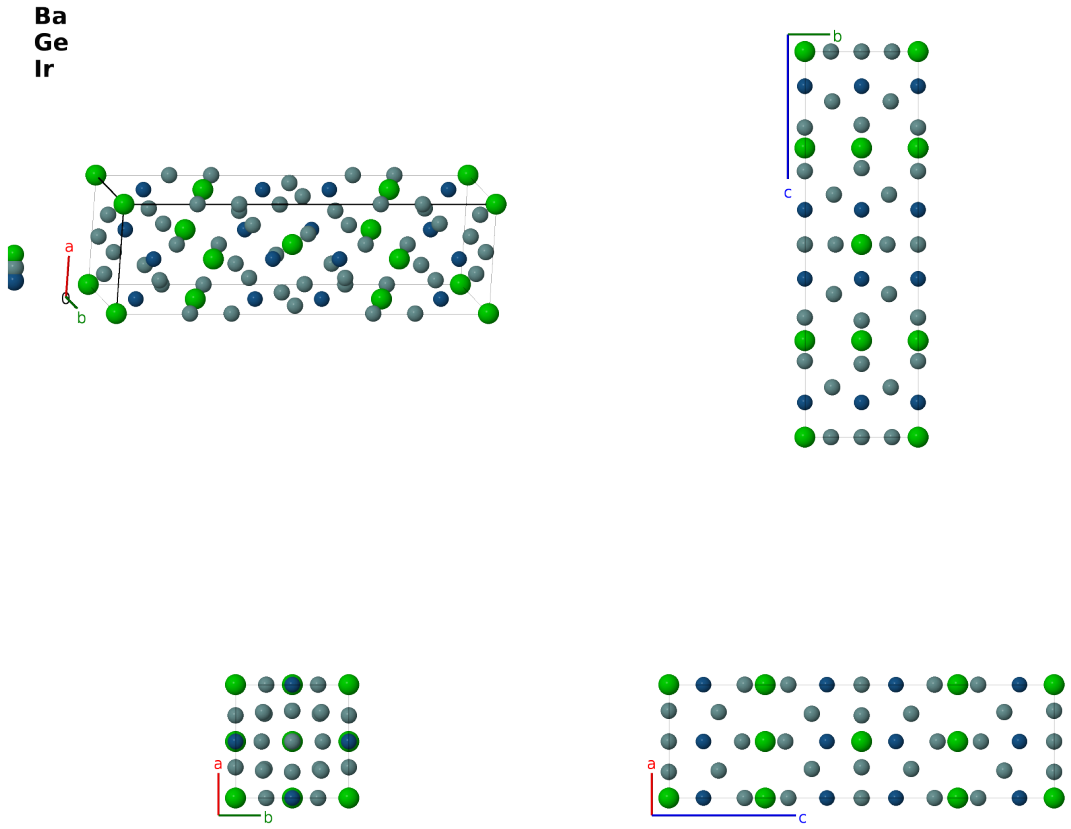
https://aflow.org/prototype-encyclopedia/SQXH

https://aflow.org/prototype-encyclopedia/A3B16C4_tI46_139_ad_2ejm_g2-001



Prototype	$Ba_3Ge_{16}Ir_4$
AFLOW prototype label	A3B16C4_tI46_139_ad_2ejm_g2-001
ICSD	194235
CCDC	1702931
Pearson symbol	tI46
Space group number	139

Space group symbol $I4/mmm$

AFLOW prototype command `aflow --proto=A3B16C4_tI46_139_ad_2ejm_g2-001 --params=`$a, c/a, z_3, z_4, z_5, x_6, x_7, z_7$

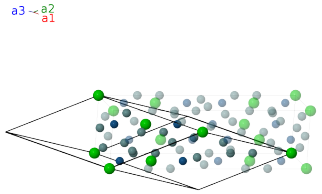
Other compounds with this structure

$Ba_3Rh_4Ge_{16}$

- $BaIr_2Ge_7$ and $Ba_3Ir_4Ge_{16}$ are structures with the barium atoms surrounded by germanium rings and germanium-iridium cages. They are superconducting at 2.5 and 5.2K, respectively.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ba I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ba II
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ba II
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Ge I
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Ge I
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	Ge II
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	Ge II
$\mathbf{B_8}$	=	$\left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8g)	Ir I
$\mathbf{B_9}$	=	$z_5\,\mathbf{a}_1 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(8g)	Ir I
$\mathbf{B_{10}}$	=	$-\left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8g)	Ir I
$\mathbf{B_{11}}$	=	$-z_5\,\mathbf{a}_1 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_5\,\hat{\mathbf{z}}$	(8g)	Ir I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(8j)	Ge III
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(8j)	Ge III
$\mathbf{B_{14}}$	=	$x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}}$	(8j)	Ge III
$\mathbf{B_{15}}$	=	$-x_6\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}}$	(8j)	Ge III
$\mathbf{B_{16}}$	=	$(x_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + 2x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{17}}$	=	$-(x_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - 2x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{18}}$	=	$(x_7 + z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2$	=	$-ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV

$\mathbf{B_{19}}$	=	$-(x_7 - z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2$	=	$ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{20}}$	=	$(x_7 - z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2$	=	$-ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{21}}$	=	$-(x_7 + z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2$	=	$ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{22}}$	=	$(x_7 - z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + 2x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{23}}$	=	$-(x_7 + z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - 2x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV

References

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[1] C. Pei, T. Ying, Y. Zhao, L. Gao, W. Cao, C. Li, H. Hosono, and Y. Qi, *Pressure-induced reemergence of superconductivity in $BaIr_2Ge_7$ and $Ba_3Ir_4Ge_{16}$ with cage structures*, Matter Radiat. Extremes **7**, 038404 (2022), doi:10.1063/5.0088235.

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