$BaIr_2Ge_7$ Structure: AB9C2_oC96_65_acg_ghoq3r_2g2h-001

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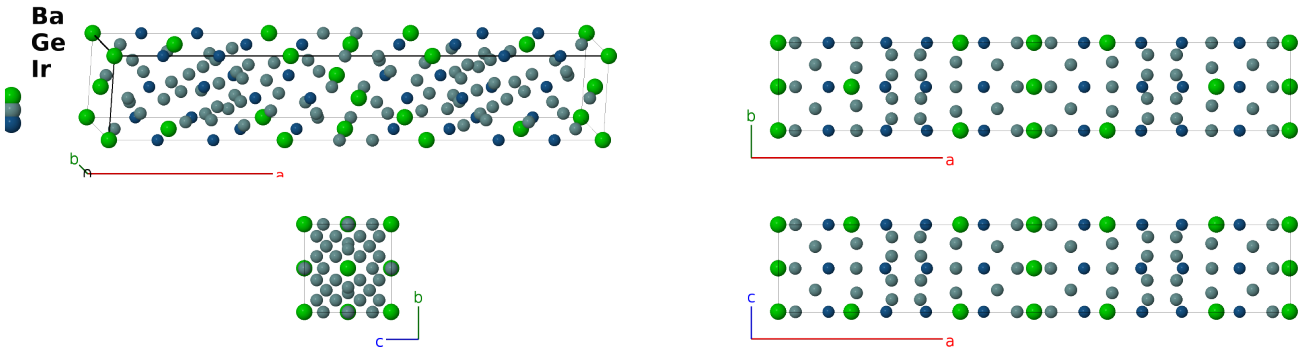
https://aflow.org/prototype-encyclopedia/FS4Q

https://aflow.org/prototype-encyclopedia/AB9C2_oC96_65_acg_ghoq3r_2g2h-001

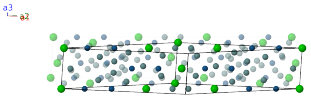


Prototype	$BaGe_7Ir_2$
AFLOW prototype label	AB9C2_oC96_65_acg_ghoq3r_2g2h-001
ICSD	194234
CCDC	1702930
Pearson symbol	oC96
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=AB9C2_oC96_65_acg_ghoq3r_2g2h-001 --params=`$a, b/a, c/a, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, z_{10}, x_{11}, y_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}$

- $BaIr_2Ge_7$ 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.
- (Ishida, 2014), wishing to present the structure with the long axis in the $\hat{z}$ direction, give the structural data for $BaIr_2Ge_7$ in the $Ammm$ setting of space group #65. We used AFLOW to transform this to the standard $Cmmm$ setting. This rotates the lattice 90° about the y-axis. In addition the origin was translated by $1/2\,\mathrm{b}\,\hat{y}$, moving the first barium atom from the (2b) site to the origin at the (2a) site.
- The Ge VI and Ge VII (16r) sites are only half-occupied, leading to the observed stoichiometry.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ba I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}}$	(4g)	Ba III
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(4g)	Ba III
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}}$	(4g)	Ge I
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}$	(4g)	Ge I
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}}$	(4g)	Ir I
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}}$	(4g)	Ir I
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2$	=	$ax_6\,\hat{\mathbf{x}}$	(4g)	Ir II
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2$	=	$-ax_6\,\hat{\mathbf{x}}$	(4g)	Ir II
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ge II
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ge II
$\mathbf{B_{13}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ir III
$\mathbf{B_{14}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ir III
$\mathbf{B_{15}}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ir IV
$\mathbf{B_{16}}$	=	$-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ir IV
$\mathbf{B_{17}}$	=	$x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + cz_{10}\,\hat{\mathbf{z}}$	(8o)	Ge III
$\mathbf{B_{18}}$	=	$-x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} + cz_{10}\,\hat{\mathbf{z}}$	(8o)	Ge III
$\mathbf{B_{19}}$	=	$-x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - cz_{10}\,\hat{\mathbf{z}}$	(8o)	Ge III
$\mathbf{B_{20}}$	=	$x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} - cz_{10}\,\hat{\mathbf{z}}$	(8o)	Ge III
$\mathbf{B_{21}}$	=	$(x_{11} - y_{11})\,\mathbf{a}_1 +$ $(x_{11} + y_{11})\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8q)	Ge IV
$\mathbf{B_{22}}$	=	$-(x_{11} - y_{11})\,\mathbf{a}_1 -$ $(x_{11} + y_{11})\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8q)	Ge IV
$\mathbf{B_{23}}$	=	$-(x_{11} + y_{11})\,\mathbf{a}_1 -$ $(x_{11} - y_{11})\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_{11}\,\hat{\mathbf{x}} + by_{11}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8q)	Ge IV
$\mathbf{B_{24}}$	=	$(x_{11} + y_{11})\,\mathbf{a}_1 +$ $(x_{11} - y_{11})\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_{11}\,\hat{\mathbf{x}} - by_{11}\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8q)	Ge IV
$\mathbf{B_{25}}$	=	$(x_{12} - y_{12})\,\mathbf{a}_1 +$ $(x_{12} + y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(16r)	Ge V
$\mathbf{B_{26}}$	=	$-(x_{12} - y_{12})\,\mathbf{a}_1 -$ $(x_{12} + y_{12})\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}} - by_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(16r)	Ge V
$\mathbf{B_{27}}$	=	$-(x_{12} + y_{12})\,\mathbf{a}_1 -$ $(x_{12} - y_{12})\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}} + by_{12}\,\hat{\mathbf{y}} - cz_{12}\,\hat{\mathbf{z}}$	(16r)	Ge V

$\mathbf{B_{28}}$	=	$(x_{12}+y_{12})\,\mathbf{a}_1+(x_{12}-y_{12})\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}}$	(16r)	Ge V
$\mathbf{B_{29}}$	=	$-(x_{12}-y_{12})\,\mathbf{a}_1-(x_{12}+y_{12})\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}}$	(16r)	Ge V
$\mathbf{B_{30}}$	=	$(x_{12}-y_{12})\,\mathbf{a}_1+(x_{12}+y_{12})\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}}$	(16r)	Ge V
$\mathbf{B_{31}}$	=	$(x_{12}+y_{12})\,\mathbf{a}_1+(x_{12}-y_{12})\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3$	=	$ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(16r)	Ge V
$\mathbf{B_{32}}$	=	$-(x_{12}+y_{12})\,\mathbf{a}_1-(x_{12}-y_{12})\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(16r)	Ge V
$\mathbf{B_{33}}$	=	$(x_{13}-y_{13})\,\mathbf{a}_1+(x_{13}+y_{13})\,\mathbf{a}_2+z_{13}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}}$	(16r)	Ge VI
$\mathbf{B_{34}}$	=	$-(x_{13}-y_{13})\,\mathbf{a}_1-(x_{13}+y_{13})\,\mathbf{a}_2+z_{13}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}}$	(16r)	Ge VI
$\mathbf{B_{35}}$	=	$-(x_{13}+y_{13})\,\mathbf{a}_1-(x_{13}-y_{13})\,\mathbf{a}_2-z_{13}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}-cz_{13}\,\hat{\mathbf{z}}$	(16r)	Ge VI
$\mathbf{B_{36}}$	=	$(x_{13}+y_{13})\,\mathbf{a}_1+(x_{13}-y_{13})\,\mathbf{a}_2-z_{13}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}-cz_{13}\,\hat{\mathbf{z}}$	(16r)	Ge VI
$\mathbf{B_{37}}$	=	$-(x_{13}-y_{13})\,\mathbf{a}_1-(x_{13}+y_{13})\,\mathbf{a}_2-z_{13}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}-cz_{13}\,\hat{\mathbf{z}}$	(16r)	Ge VI
$\mathbf{B_{38}}$	=	$(x_{13}-y_{13})\,\mathbf{a}_1+(x_{13}+y_{13})\,\mathbf{a}_2-z_{13}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}-cz_{13}\,\hat{\mathbf{z}}$	(16r)	Ge VI
$\mathbf{B_{39}}$	=	$(x_{13}+y_{13})\,\mathbf{a}_1+(x_{13}-y_{13})\,\mathbf{a}_2+z_{13}\,\mathbf{a}_3$	=	$ax_{13}\,\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}}$	(16r)	Ge VI
$\mathbf{B_{40}}$	=	$-(x_{13}+y_{13})\,\mathbf{a}_1-(x_{13}-y_{13})\,\mathbf{a}_2+z_{13}\,\mathbf{a}_3$	=	$-ax_{13}\,\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}}$	(16r)	Ge VI
$\mathbf{B_{41}}$	=	$(x_{14}-y_{14})\,\mathbf{a}_1+(x_{14}+y_{14})\,\mathbf{a}_2+z_{14}\,\mathbf{a}_3$	=	$ax_{14}\,\hat{\mathbf{x}}+by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(16r)	Ge VII
$\mathbf{B_{42}}$	=	$-(x_{14}-y_{14})\,\mathbf{a}_1-(x_{14}+y_{14})\,\mathbf{a}_2+z_{14}\,\mathbf{a}_3$	=	$-ax_{14}\,\hat{\mathbf{x}}-by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(16r)	Ge VII
$\mathbf{B_{43}}$	=	$-(x_{14}+y_{14})\,\mathbf{a}_1-(x_{14}-y_{14})\,\mathbf{a}_2-z_{14}\,\mathbf{a}_3$	=	$-ax_{14}\,\hat{\mathbf{x}}+by_{14}\,\hat{\mathbf{y}}-cz_{14}\,\hat{\mathbf{z}}$	(16r)	Ge VII
$\mathbf{B_{44}}$	=	$(x_{14}+y_{14})\,\mathbf{a}_1+(x_{14}-y_{14})\,\mathbf{a}_2-z_{14}\,\mathbf{a}_3$	=	$ax_{14}\,\hat{\mathbf{x}}-by_{14}\,\hat{\mathbf{y}}-cz_{14}\,\hat{\mathbf{z}}$	(16r)	Ge VII
$\mathbf{B_{45}}$	=	$-(x_{14}-y_{14})\,\mathbf{a}_1-(x_{14}+y_{14})\,\mathbf{a}_2-z_{14}\,\mathbf{a}_3$	=	$-ax_{14}\,\hat{\mathbf{x}}-by_{14}\,\hat{\mathbf{y}}-cz_{14}\,\hat{\mathbf{z}}$	(16r)	Ge VII
$\mathbf{B_{46}}$	=	$(x_{14}-y_{14})\,\mathbf{a}_1+(x_{14}+y_{14})\,\mathbf{a}_2-z_{14}\,\mathbf{a}_3$	=	$ax_{14}\,\hat{\mathbf{x}}+by_{14}\,\hat{\mathbf{y}}-cz_{14}\,\hat{\mathbf{z}}$	(16r)	Ge VII
$\mathbf{B_{47}}$	=	$(x_{14}+y_{14})\,\mathbf{a}_1+(x_{14}-y_{14})\,\mathbf{a}_2+z_{14}\,\mathbf{a}_3$	=	$ax_{14}\,\hat{\mathbf{x}}-by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(16r)	Ge VII
$\mathbf{B_{48}}$	=	$-(x_{14}+y_{14})\,\mathbf{a}_1-(x_{14}-y_{14})\,\mathbf{a}_2+z_{14}\,\mathbf{a}_3$	=	$-ax_{14}\,\hat{\mathbf{x}}+by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(16r)	Ge VII

References

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