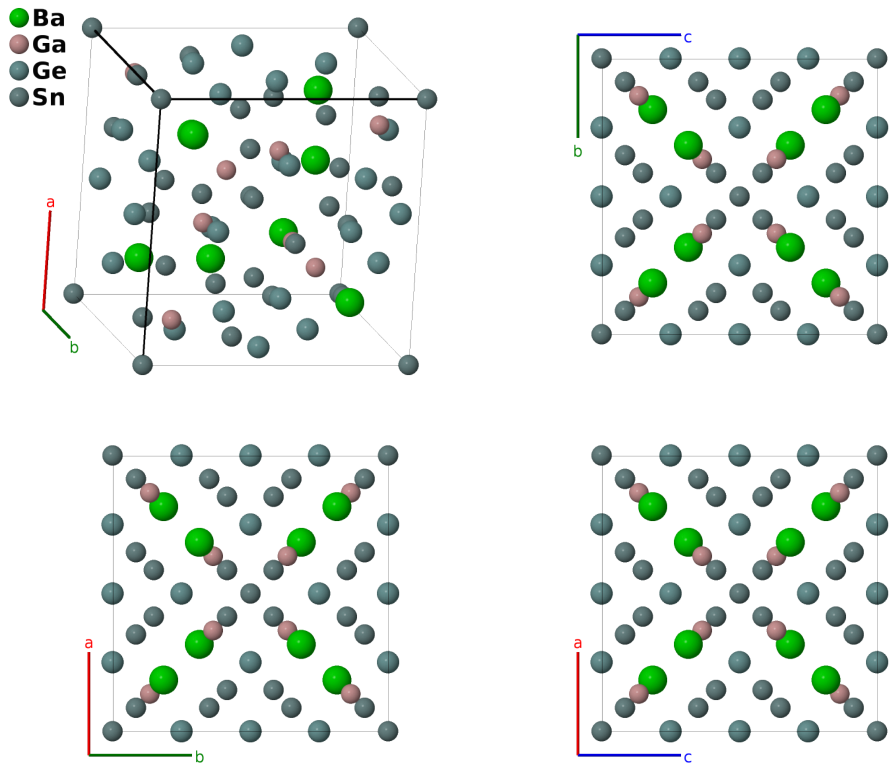
α-$Ba_8Ga_{16}Sn_{30}$ Clathrate Structure: A4B4C6D13_cI54_217_c_c_d_ag-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

---

https://aflow.org/p/YXNP

https://aflow.org/p/A4B4C6D13_cI54_217_c_c_d_ag-001



Prototype $Ba_4Ga_8Sn_{15}$

AFLOW prototype label A4B4C6D13_cI54_217_c_c_d_ag-001

ICSD none

Pearson symbol cI54

Space group number 217

Space group symbol $I\bar{4}3m$

AFLOW prototype command `aflow --proto=A4B4C6D13_cI54_217_c_c_d_ag-001`
`--params=`a, x_2, x_3, x_5, z_5

Other compounds with this structure
$Ba_8Ga_{16}Ge_{30}$

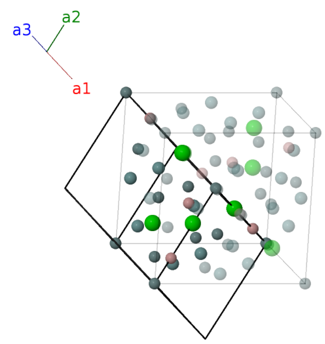
- There is a considerable amount of disorder in this system:
  - The (2a) site is 84.2% tin and 15.8% gallium. We label it Sn.

  - The first (8c) site is pure barium, labeled Ba.
  - The second (8c) site is 76.6% gallium and 23.4% tin, and is labeled Ga.
  - The (12d) site is 81.60% tin and 18.4% gallium. We label this as germanium, Ge, since that is another possible component of this compound and to avoid confusion with the other tin/gallium sites.
  - The (24g) site is 68.6% gallium and 31.4% tin, and is labeled Sn.

- The occupation of each of the Sn/Ga sites can be varied during crystal growth, and controls the semiconducting behavior of the sample (Avila, 2006).
- (Aliva, 2008) showed that this compound also exists as β-$Ba_8Ga_{16}Sn_{30}$, another clathrate structure.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Sn I
$\mathbf{B_2}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Ba I
$\mathbf{B_3}$	=	$-2x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8c)	Ba I
$\mathbf{B_4}$	=	$-2x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Ba I
$\mathbf{B_5}$	=	$-2x_2\,\mathbf{a}_1$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8c)	Ba I
$\mathbf{B_6}$	=	$2x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_7}$	=	$-2x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_8}$	=	$-2x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_9}$	=	$-2x_3\,\mathbf{a}_1$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(8c)	Ga I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(12d)	Ge I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B_{12}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B_{13}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(12d)	Ge I
$\mathbf{B_{14}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B_{15}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12d)	Ge I
$\mathbf{B_{16}}$	=	$(x_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + 2x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{17}}$	=	$-(x_5 - z_5)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - 2x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{18}}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{19}}$	=	$-(x_5 + z_5)\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(24g)	Sn II

$\mathbf{B_{20}}$	=	$2x_5\,\mathbf{a}_1 + (x_5+z_5)\,\mathbf{a}_2 + (x_5+z_5)\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{21}}$	=	$-2x_5\,\mathbf{a}_1 - (x_5-z_5)\,\mathbf{a}_2 - (x_5-z_5)\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{22}}$	=	$(x_5-z_5)\,\mathbf{a}_2 - (x_5+z_5)\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{23}}$	=	$-(x_5+z_5)\,\mathbf{a}_2 + (x_5-z_5)\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{24}}$	=	$(x_5+z_5)\,\mathbf{a}_1 + 2x_5\,\mathbf{a}_2 + (x_5+z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{25}}$	=	$-(x_5-z_5)\,\mathbf{a}_1 - 2x_5\,\mathbf{a}_2 - (x_5-z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{26}}$	=	$-(x_5+z_5)\,\mathbf{a}_1 + (x_5-z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(24g)	Sn II
$\mathbf{B_{27}}$	=	$(x_5-z_5)\,\mathbf{a}_1 - (x_5+z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(24g)	Sn II

References

[1] M. A. Avila, K. Suekuni, K. Umeo, H. Fukuoka, S. Yamanaka, and T. Takabatake, *Glasslike versus crystalline thermal conductivity in carrier-tuned $Ba_8Ga_{16}X_{30}$ clathrates (X=Ge,Sn)*, Phys. Rev. B **74**, 125109 (2006), doi:10.1103/PhysRevB.74.125109.

[2] M. A. Avila, K. Suekuni, K. Umeo, H. Fukuoka, S. Yamanaka, and T. Takabatake, *$Ba_8Ga_{16}Sn_{30}$ with type-I clathrate structure: Drastic suppression of heat conduction*, Appl. Phys. Lett. **92**, 041901 (2007), doi:10.1063/1.2831926.

Found in

[1] M. A. Avila, K. Suekuni, K. Umeo, H. Fukuoka, S. Yamanaka, and T. Takabatake, *$Ba_8Ga_{16}Sn_{30}$ with type-I clathrate structure: Drastic suppression of heat conduction*, Appl. Phys. Lett. **92**, 041901 (2007), doi:10.1063/1.2831926.