α-Sm$_3$Ge$_5$ (High-temperature) Structure: A5B3_hP16_190_bch_g-001
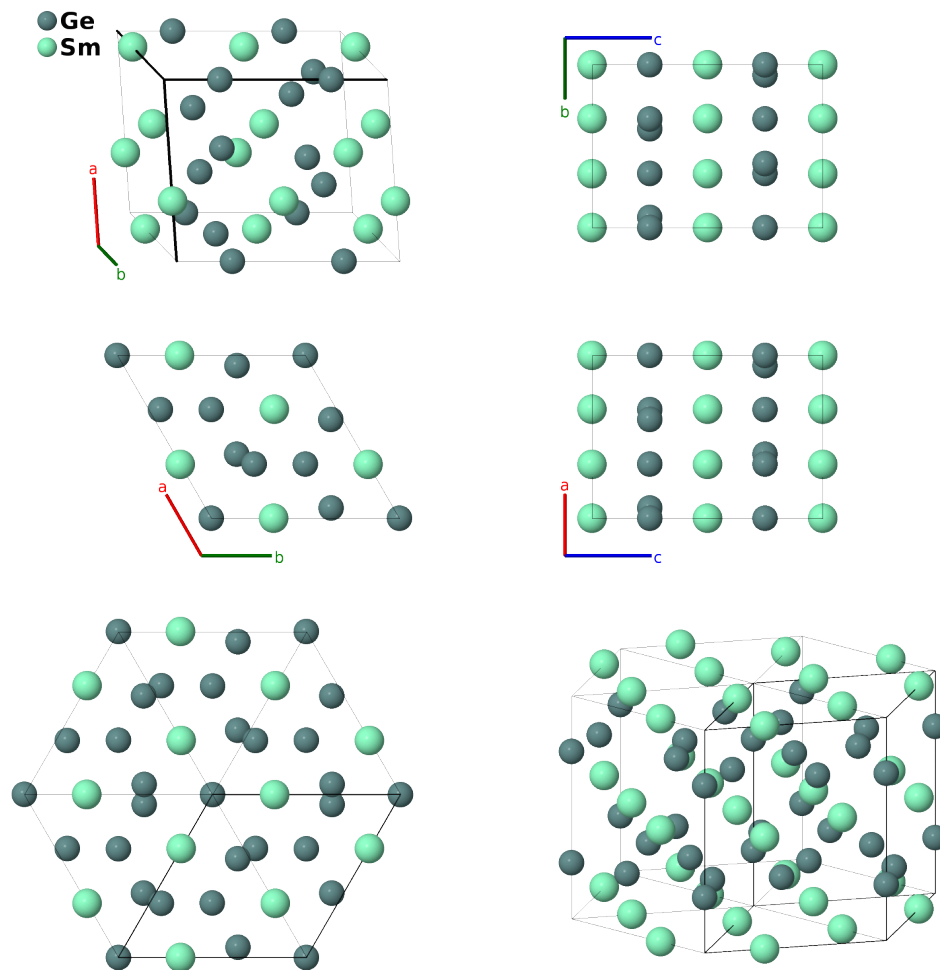
This structure originally had the label `A5B3_hP16_190_bdh_g`. Calls to that address will be redirected here.

https://aflow.org/p/PJF4

https://aflow.org/p/A5B3_hP16_190_bch_g-001

Prototype	Ge$_5$Sm$_3$
AFLOW prototype label	A5B3_hP16_190_bch_g-001
ICSD	416581
Pearson symbol	hP16
Space group number	190
Space group symbol	$P\bar{6}2c$
AFLOW prototype command	aflow --proto=A5B3_hP16_190_bch_g-001 --params=$a, c/a, x_3, x_4, y_4$

1

Hexagonal primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
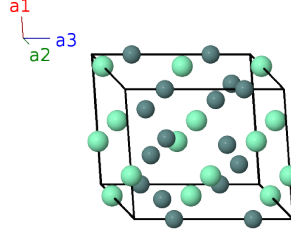
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$\tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2b)	Ge I
$\mathbf{B_2}$	$=$	$\tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2b)	Ge I
$\mathbf{B_3}$	$=$	$\tfrac{1}{3}\mathbf{a_1} + \tfrac{2}{3}\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Ge II
$\mathbf{B_4}$	$=$	$\tfrac{2}{3}\mathbf{a_1} + \tfrac{1}{3}\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Ge II
$\mathbf{B_5}$	$=$	$x_3\,\mathbf{a_1}$	$=$	$\tfrac{1}{2}ax_3\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6g)	Sm I
$\mathbf{B_6}$	$=$	$x_3\,\mathbf{a_2}$	$=$	$\tfrac{1}{2}ax_3\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(6g)	Sm I
$\mathbf{B_7}$	$=$	$-x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2}$	$=$	$-ax_3\,\hat{\mathbf{x}}$	(6g)	Sm I
$\mathbf{B_8}$	$=$	$x_3\,\mathbf{a_1} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}ax_3\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Sm I
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$\tfrac{1}{2}ax_3\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Sm I
$\mathbf{B_{10}}$	$=$	$-x_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} + \tfrac{1}{2}\mathbf{a_3}$	$=$	$-ax_3\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Sm I
$\mathbf{B_{11}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B_{12}}$	$=$	$-y_4\,\mathbf{a_1} + (x_4 - y_4)\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B_{13}}$	$=$	$-(x_4 - y_4)\,\mathbf{a_1} - x_4\,\mathbf{a_2} + \tfrac{1}{4}\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B_{14}}$	$=$	$y_4\,\mathbf{a_1} + x_4\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B_{15}}$	$=$	$(x_4 - y_4)\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ge III
$\mathbf{B_{16}}$	$=$	$-x_4\,\mathbf{a_1} - (x_4 - y_4)\,\mathbf{a_2} + \tfrac{3}{4}\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Ge III

References

[1] P. H. Tobash, D. Lins, S. Bobev, N. Hur, J. D. Thompson, and J. L. Sarrao, *Vacancy Ordering in $SmGe_{2-x}$ and $GdGe_{2-x}$ (x = 0.33): Structure and Properties of Two Sm_3Ge_5 Polymorphs and of Gd_3Ge_5*, Inorg. Chem. **45**, 7286–7294 (2006), doi:10.1021/ic060913f.

Found in

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