$Sc_{11}Al_2Ge_8$ Structure: A2B8C11_tI84_139_h_deim_eh2n-001

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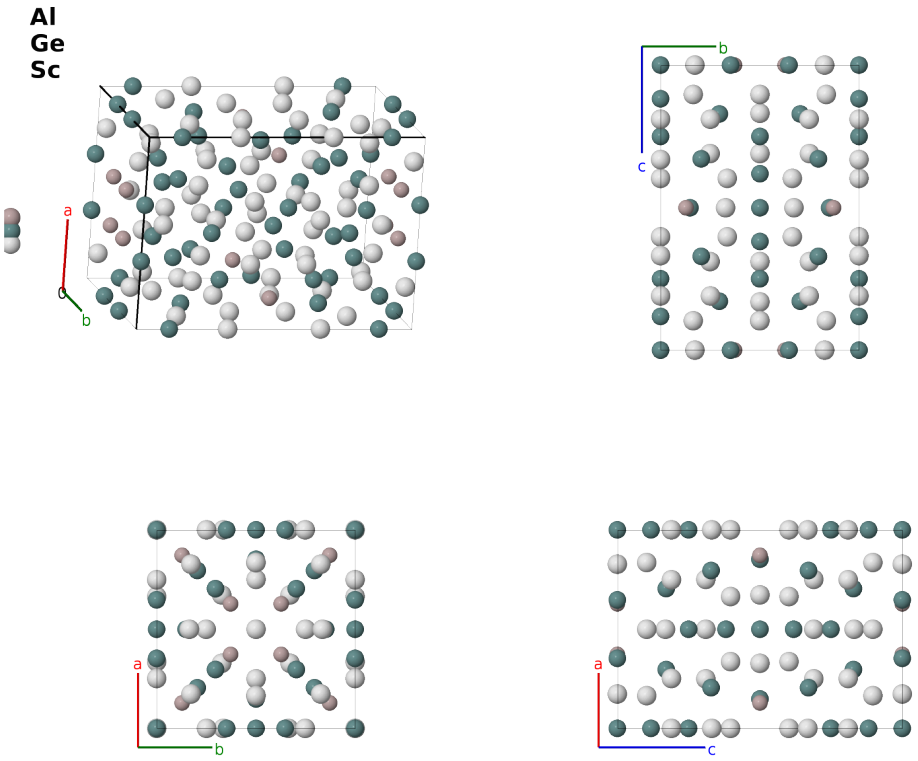
https://aflow.org/prototype-encyclopedia/DVM5

https://aflow.org/prototype-encyclopedia/A2B8C11_tI84_139_h_deim_eh2n-001



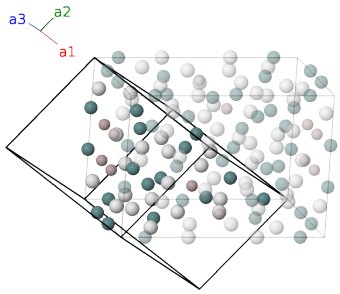
Prototype	$Al_2Ge_8Sc_{11}$
AFLOW prototype label	A2B8C11_tI84_139_h_deim_eh2n-001
ICSD	184236
CCDC	1693480
Pearson symbol	tI84
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A2B8C11_tI84_139_h_deim_eh2n-001 --params=`$a, c/a, z_2, z_3, x_4, x_5, x_6, x_7, z_7, y_8, z_8, y_9, z_9$

Other compounds with this structure
$Er_{11}Al_2Ge_8$, $Gd_{11}In_2Ge_8$, $Yb_{11}Sn_2Bi_8$

- This is a tenary form of $Ho_{11}Ge_{10}$. The ICSD lists all these compounds using the $Ho_{11}Ge_{10}$ prototype. We arbitrarily chose $Sc_{11}Al_2Ge_8$ as the prototype.
- $Tb_{11}Si_4In_6$ is a second ternary form of $Ho_{11}Ge_{10}$.
- The AFLOW standard labeling algorithm shifts the origin by (0.5 a, 0.5 b, 0), moving the Ge III atom from the published (8j) Wyckoff position to (8i).

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
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ge I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ge I
$\mathbf{B_3}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(4e)	Ge II
$\mathbf{B_4}$	=	$-z_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$	=	$-cz_2\,\hat{\mathbf{z}}$	(4e)	Ge II
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Sc I
$\mathbf{B_6}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Sc I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	Al I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	Al I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	Al I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	Al I
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + 2x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(8h)	Sc II
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - 2x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(8h)	Sc II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(8h)	Sc II
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(8h)	Sc II
$\mathbf{B_{15}}$	=	$x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}$	(8i)	Ge III
$\mathbf{B_{16}}$	=	$-x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}$	(8i)	Ge III
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{y}}$	(8i)	Ge III
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{y}}$	(8i)	Ge III
$\mathbf{B_{19}}$	=	$(x_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + 2x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV

$\mathbf{B_{20}}$	=	$-(x_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - 2x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{21}}$	=	$(x_7 + z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2$	=	$-ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{22}}$	=	$-(x_7 - z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2$	=	$ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{23}}$	=	$(x_7 - z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2$	=	$-ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{24}}$	=	$-(x_7 + z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2$	=	$ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{25}}$	=	$(x_7 - z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + 2x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{26}}$	=	$-(x_7 + z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - 2x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(16m)	Ge IV
$\mathbf{B_{27}}$	=	$(y_8 + z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(16n)	Sc III
$\mathbf{B_{28}}$	=	$-(y_8 - z_8)\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - y_8\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(16n)	Sc III
$\mathbf{B_{29}}$	=	$z_8\,\mathbf{a}_1 - (y_8 - z_8)\,\mathbf{a}_2 - y_8\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(16n)	Sc III
$\mathbf{B_{30}}$	=	$z_8\,\mathbf{a}_1 + (y_8 + z_8)\,\mathbf{a}_2 + y_8\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(16n)	Sc III
$\mathbf{B_{31}}$	=	$(y_8 - z_8)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + y_8\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(16n)	Sc III
$\mathbf{B_{32}}$	=	$-(y_8 + z_8)\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - y_8\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(16n)	Sc III
$\mathbf{B_{33}}$	=	$-z_8\,\mathbf{a}_1 + (y_8 - z_8)\,\mathbf{a}_2 + y_8\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}}$	(16n)	Sc III
$\mathbf{B_{34}}$	=	$-z_8\,\mathbf{a}_1 - (y_8 + z_8)\,\mathbf{a}_2 - y_8\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}} - cz_8\,\hat{\mathbf{z}}$	(16n)	Sc III
$\mathbf{B_{35}}$	=	$(y_9 + z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 + y_9\,\mathbf{a}_3$	=	$ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(16n)	Sc IV
$\mathbf{B_{36}}$	=	$-(y_9 - z_9)\,\mathbf{a}_1 + z_9\,\mathbf{a}_2 - y_9\,\mathbf{a}_3$	=	$-ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(16n)	Sc IV
$\mathbf{B_{37}}$	=	$z_9\,\mathbf{a}_1 - (y_9 - z_9)\,\mathbf{a}_2 - y_9\,\mathbf{a}_3$	=	$-ay_9\,\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}}$	(16n)	Sc IV
$\mathbf{B_{38}}$	=	$z_9\,\mathbf{a}_1 + (y_9 + z_9)\,\mathbf{a}_2 + y_9\,\mathbf{a}_3$	=	$ay_9\,\hat{\mathbf{x}} + cz_9\,\hat{\mathbf{z}}$	(16n)	Sc IV
$\mathbf{B_{39}}$	=	$(y_9 - z_9)\,\mathbf{a}_1 - z_9\,\mathbf{a}_2 + y_9\,\mathbf{a}_3$	=	$ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(16n)	Sc IV
$\mathbf{B_{40}}$	=	$-(y_9 + z_9)\,\mathbf{a}_1 - z_9\,\mathbf{a}_2 - y_9\,\mathbf{a}_3$	=	$-ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(16n)	Sc IV
$\mathbf{B_{41}}$	=	$-z_9\,\mathbf{a}_1 + (y_9 - z_9)\,\mathbf{a}_2 + y_9\,\mathbf{a}_3$	=	$ay_9\,\hat{\mathbf{x}} - cz_9\,\hat{\mathbf{z}}$	(16n)	Sc IV
$\mathbf{B_{42}}$	=	$-z_9\,\mathbf{a}_1 - (y_9 + z_9)\,\mathbf{a}_2 - y_9\,\mathbf{a}_3$	=	$-ay_9\,\hat{\mathbf{x}} - cz_9\,\hat{\mathbf{z}}$	(16n)	Sc IV

References

[1] J. T. Zhao and E. Parthé, *$Sc_{11}Al_2Ge_8$, a ternary substitution variant of the tetragonal $Ho_{11}Ge_{10}$ type*, Acta Crystallogr. Sect. C **47**, 4–6 (1991), doi:10.1107/S0108270190007314.

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