

La₄Ge₃S₁₂ Structure:

A3B4C12_hR38_161_b_ab_4b-001

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<https://aflow.org/prototype-encyclopedia/25NH>

https://aflow.org/prototype-encyclopedia/A3B4C12_hR38_161_b_ab_4b-001

Prototype	Ge ₃ La ₄ S ₁₂
AFLOW prototype label	A3B4C12_hR38_161_b_ab_4b-001
ICSD	2046
CCDC	1591996
Pearson symbol	hR38
Space group number	161
Space group symbol	<i>R</i> 3 <i>c</i>
AFLOW prototype command	aflow --proto=A3B4C12_hR38_161_b_ab_4b-001 --params= <i>a</i> , <i>c/a</i> , <i>x</i> ₁ , <i>x</i> ₂ , <i>y</i> ₂ , <i>z</i> ₂ , <i>x</i> ₃ , <i>y</i> ₃ , <i>z</i> ₃ , <i>x</i> ₄ , <i>y</i> ₄ , <i>z</i> ₄ , <i>x</i> ₅ , <i>y</i> ₅ , <i>z</i> ₅ , <i>x</i> ₆ , <i>y</i> ₆ , <i>z</i> ₆ , <i>x</i> ₇ , <i>y</i> ₇ , <i>z</i> ₇

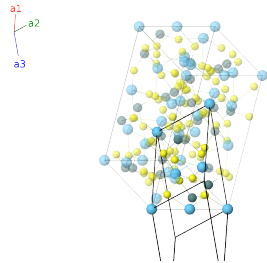
Other compounds with this structure

Ce₄Ge₃S₁₂, Ce₄Si₃S₁₂, Fe₄C₃O₁₂, Gd₄Ge₃S₁₂, Gd₄Si₃S₁₂, Nd₄Ge₃S₁₂, Nd₄Si₃S₁₂, Pr₄Ge₃S₁₂, Pr₄Si₃S₁₂, Sm₄Ge₃S₁₂, Sm₄Si₃S₁₂

- Space group *R*3*c* #161 is polar and has no fixed origin along the *z*-axis. We follow (Mazurier, 1974) and put one of the La (2a) atoms at origin, setting *x*₁ = 0.

Rhombohedral primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
 \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B₁	=	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$c x_1 \hat{\mathbf{z}}$	(2a) La I
B₂	=	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + (x_1 + \frac{1}{2}) \mathbf{a}_3$	=	$c (x_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a) La I

$\mathbf{B}_{26}$	$=$	$\begin{pmatrix} x_5 + \frac{1}{2} \\ y_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} z_5 + \frac{1}{2} \\ y_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{6}c(2x_5 + 2y_5 + 2z_5 + 3) \hat{\mathbf{z}}$	(6b)	S II
$\mathbf{B}_{27}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6b)	S III
$\mathbf{B}_{28}$	$=$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6b)	S III
$\mathbf{B}_{29}$	$=$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6b)	S III
$\mathbf{B}_{30}$	$=$	$\begin{pmatrix} z_6 + \frac{1}{2} \\ x_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_6 + \frac{1}{2} \\ x_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 + 3) \hat{\mathbf{z}}$	(6b)	S III
$\mathbf{B}_{31}$	$=$	$\begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 + 3) \hat{\mathbf{z}}$	(6b)	S III
$\mathbf{B}_{32}$	$=$	$\begin{pmatrix} x_6 + \frac{1}{2} \\ y_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} z_6 + \frac{1}{2} \\ y_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{6}c(2x_6 + 2y_6 + 2z_6 + 3) \hat{\mathbf{z}}$	(6b)	S III
$\mathbf{B}_{33}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6b)	S IV
$\mathbf{B}_{34}$	$=$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6b)	S IV
$\mathbf{B}_{35}$	$=$	$y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6b)	S IV
$\mathbf{B}_{36}$	$=$	$\begin{pmatrix} z_7 + \frac{1}{2} \\ x_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_7 + \frac{1}{2} \\ x_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 + 3) \hat{\mathbf{z}}$	(6b)	S IV
$\mathbf{B}_{37}$	$=$	$\begin{pmatrix} y_7 + \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_7 + \frac{1}{2} \\ z_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 + 3) \hat{\mathbf{z}}$	(6b)	S IV
$\mathbf{B}_{38}$	$=$	$\begin{pmatrix} x_7 + \frac{1}{2} \\ y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} z_7 + \frac{1}{2} \\ y_7 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{6}c(2x_7 + 2y_7 + 2z_7 + 3) \hat{\mathbf{z}}$	(6b)	S IV

References

- [1] A. Mazurier and J. Etienne, *Structure cristalline de $\text{La}_4\text{Ge}_3\text{S}_{12}$* , Acta Crystallogr. Sect. B **30**, 759–762 (1974), doi:10.1107/S0567740874003657.

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