

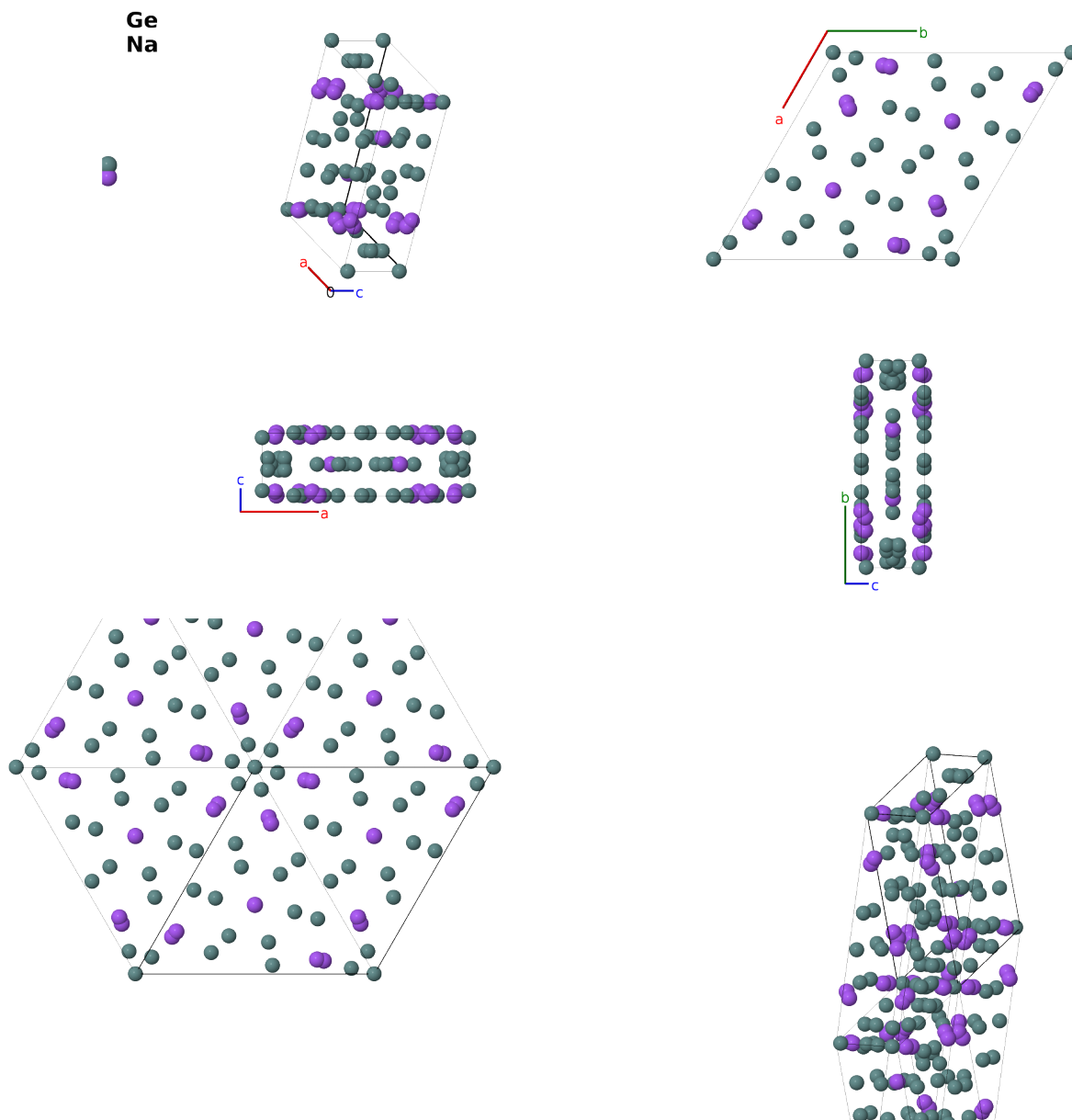
Na₄Ge₁₃ Structure: A19B10_hP58_175_e2j2kl_djl-001

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<https://aflow.org/prototype-encyclopedia/XPLN>

https://aflow.org/prototype-encyclopedia/A19B10_hP58_175_e2j2kl_djl-001



Prototype

Ge₁₃Na₄

AFLOW prototype label

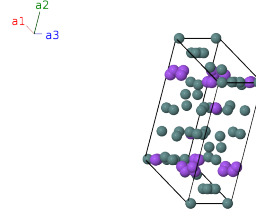
A19B10_hP58_175_e2j2kl_djl-001

ICSD	256042
CCDC	1585853
Pearson symbol	hP58
Space group number	175
Space group symbol	$P6/m$
AFLOW prototype command	<code>aflow --proto=A19B10_hP58_175_e2j2kl_dj1-001</code> <code>--params=a, c/a, z₂, x₃, y₃, x₄, y₄, x₅, y₅, x₆, y₆, x₇, y₇, x₈, y₈, z₈, x₉, y₉, z₉</code>

- There are a large number of vacancies in this structure leading to the composition $\text{Na}_4\text{Ge}_{13}$:
 - The Ge-I (2e) site is only occupied 25% of the time.
 - The Na-II (6j) site has 50% occupation, so that only one of each sodium doublet is occupied.
 - The Ge-VI (12l) site has 12.5% occupation.
 - The Ni-III (12) site has 25% occupation.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2d)	Na I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2d)	Na I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(2e)	Ge I
$\mathbf{B}_4$	$= -z_2 \mathbf{a}_3$	$=$	$-cz_2 \hat{\mathbf{z}}$	(2e)	Ge I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}}$	(6j)	Ge II
$\mathbf{B}_6$	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6j)	Ge II
$\mathbf{B}_7$	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}}$	(6j)	Ge II
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_3 - y_3) \hat{\mathbf{y}}$	(6j)	Ge II
$\mathbf{B}_9$	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2$	$=$	$\frac{1}{2}a (-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(6j)	Ge II
$\mathbf{B}_{10}$	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$\frac{1}{2}a (2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}}$	(6j)	Ge II
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}}$	(6j)	Ge III
$\mathbf{B}_{12}$	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(6j)	Ge III
$\mathbf{B}_{13}$	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}}$	(6j)	Ge III
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}}$	(6j)	Ge III
$\mathbf{B}_{15}$	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2$	$=$	$\frac{1}{2}a (-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(6j)	Ge III
$\mathbf{B}_{16}$	$= (x_4 - y_4) \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}}$	(6j)	Ge III

$$\mathbf{B}_{58} = -(x_9 - y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 = -\frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} \quad (121) \quad \text{Na III}$$

References

- [1] S. Stefanoski, G. J. Finkelstein, M. D. Ward, T. Zeng, K. Wei, E. S. Bullock, C. M. Beavers, H. Liu, G. S. Nolas, and T. A. Strobel, *Zintl Ions within Framework Channels: The Complex Structure and Low-Temperature Transport Properties of $\text{Na}_4\text{Ge}_{13}$* , *Inorg. Chem.* **57**, 2002–2012 (2018), doi:10.1021/acs.inorgchem.7b02914.

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