

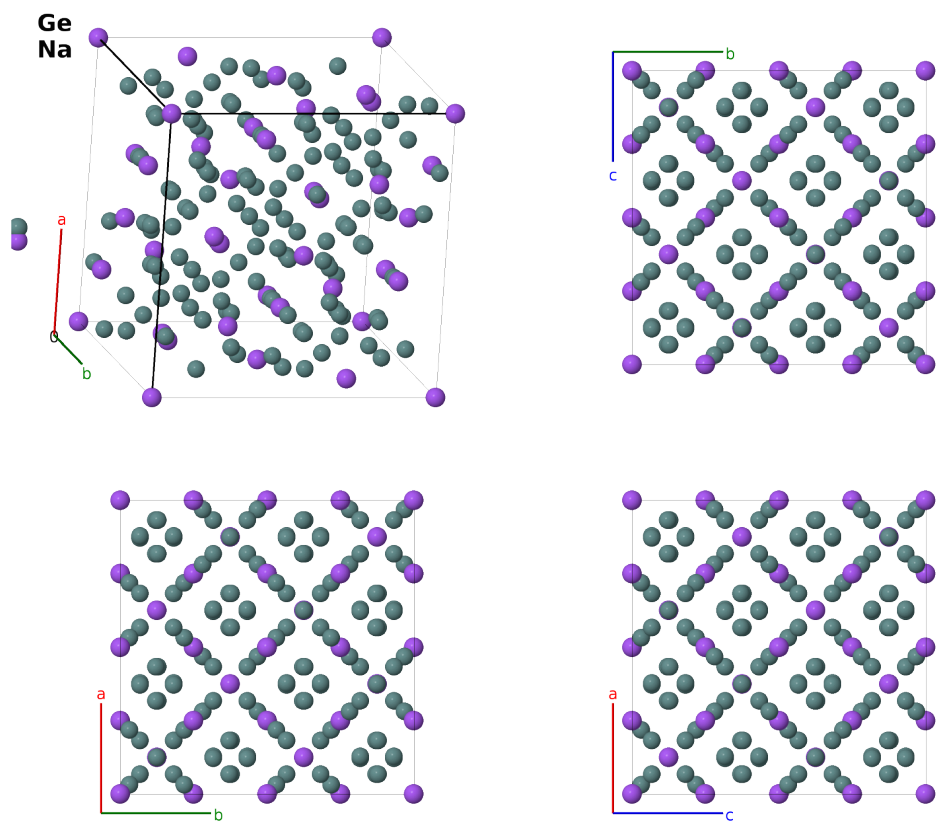
Na_{24-δ}Ge₁₃₆ Clathrate Structure: A17B3_cF160_227_aeg_bc-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/33TQ>

https://aflow.org/prototype-encyclopedia/A17B3_cF160_227_aeg_bc-001

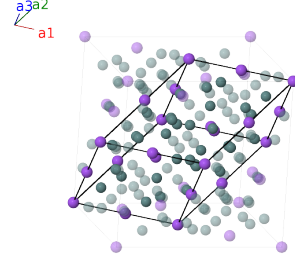


Prototype	Ge ₁₇ Na ₃
AFLOW prototype label	A17B3_cF160_227_aeg_bc-001
ICSD	113914
CCDC	2228987
Pearson symbol	cF160
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A17B3_cF160_227_aeg_bc-001</code> <code>--params=a, x₄, x₅, z₅</code>

- This is a metastable type II clathrate structure. Only 2/3 of the Na (8b) sites are occupied, making the actual composition $\text{Na}_{21.33}\text{Ge}_{136}$ ($\text{Na}_{1.253}\text{Ge}_{17}$).
- We use the Rietveld refinement data from (Feng, 2021).

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(8a)	Ge I
$\mathbf{B}_2$	$= \frac{7}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{7}{8}a\hat{\mathbf{x}} + \frac{7}{8}a\hat{\mathbf{y}} + \frac{7}{8}a\hat{\mathbf{z}}$	(8a)	Ge I
$\mathbf{B}_3$	$= \frac{3}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(8b)	Na I
$\mathbf{B}_4$	$= \frac{5}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{5}{8}a\hat{\mathbf{x}} + \frac{5}{8}a\hat{\mathbf{y}} + \frac{5}{8}a\hat{\mathbf{z}}$	(8b)	Na I
$\mathbf{B}_5$	$= 0$	$=$	0	(16c)	Na II
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(16c)	Na II
$\mathbf{B}_7$	$= \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c)	Na II
$\mathbf{B}_8$	$= \frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(16c)	Na II
$\mathbf{B}_9$	$= x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(32e)	Ge II
$\mathbf{B}_{10}$	$= x_4\mathbf{a}_1 + x_4\mathbf{a}_2 - (3x_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{4})\hat{\mathbf{x}} - a(x_4 - \frac{1}{4})\hat{\mathbf{y}} + ax_4\hat{\mathbf{z}}$	(32e)	Ge II
$\mathbf{B}_{11}$	$= x_4\mathbf{a}_1 - (3x_4 - \frac{1}{2})\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{4})\hat{\mathbf{x}} + ax_4\hat{\mathbf{y}} - a(x_4 - \frac{1}{4})\hat{\mathbf{z}}$	(32e)	Ge II
$\mathbf{B}_{12}$	$= -(3x_4 - \frac{1}{2})\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} - a(x_4 - \frac{1}{4})\hat{\mathbf{y}} - a(x_4 - \frac{1}{4})\hat{\mathbf{z}}$	(32e)	Ge II
$\mathbf{B}_{13}$	$= -x_4\mathbf{a}_1 - x_4\mathbf{a}_2 + (3x_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{4})\hat{\mathbf{x}} + a(x_4 + \frac{1}{4})\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(32e)	Ge II
$\mathbf{B}_{14}$	$= -x_4\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} - ax_4\hat{\mathbf{z}}$	(32e)	Ge II
$\mathbf{B}_{15}$	$= -x_4\mathbf{a}_1 + (3x_4 + \frac{1}{2})\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{4})\hat{\mathbf{x}} - ax_4\hat{\mathbf{y}} + a(x_4 + \frac{1}{4})\hat{\mathbf{z}}$	(32e)	Ge II
$\mathbf{B}_{16}$	$= (3x_4 + \frac{1}{2})\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} + a(x_4 + \frac{1}{4})\hat{\mathbf{y}} + a(x_4 + \frac{1}{4})\hat{\mathbf{z}}$	(32e)	Ge II
$\mathbf{B}_{17}$	$= z_5\mathbf{a}_1 + z_5\mathbf{a}_2 + (2x_5 - z_5)\mathbf{a}_3$	$=$	$ax_5\hat{\mathbf{x}} + ax_5\hat{\mathbf{y}} + az_5\hat{\mathbf{z}}$	(96g)	Ge III
$\mathbf{B}_{18}$	$= z_5\mathbf{a}_1 + z_5\mathbf{a}_2 - (2x_5 + z_5 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{4})\hat{\mathbf{x}} - a(x_5 - \frac{1}{4})\hat{\mathbf{y}} + az_5\hat{\mathbf{z}}$	(96g)	Ge III
$\mathbf{B}_{19}$	$= (2x_5 - z_5)\mathbf{a}_1 - (2x_5 + z_5 - \frac{1}{2})\mathbf{a}_2 + z_5\mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{4})\hat{\mathbf{x}} + ax_5\hat{\mathbf{y}} - a(z_5 - \frac{1}{4})\hat{\mathbf{z}}$	(96g)	Ge III
$\mathbf{B}_{20}$	$= -(2x_5 + z_5 - \frac{1}{2})\mathbf{a}_1 + (2x_5 - z_5)\mathbf{a}_2 + z_5\mathbf{a}_3$	$=$	$ax_5\hat{\mathbf{x}} - a(x_5 - \frac{1}{4})\hat{\mathbf{y}} - a(z_5 - \frac{1}{4})\hat{\mathbf{z}}$	(96g)	Ge III
$\mathbf{B}_{21}$	$= (2x_5 - z_5)\mathbf{a}_1 + z_5\mathbf{a}_2 + z_5\mathbf{a}_3$	$=$	$az_5\hat{\mathbf{x}} + ax_5\hat{\mathbf{y}} + ax_5\hat{\mathbf{z}}$	(96g)	Ge III

$$\begin{aligned}
\mathbf{B}_{22} &= -\left(2x_5 + z_5 - \frac{1}{2}\right) \mathbf{a}_1 + z_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 = az_5 \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{23} &= z_5 \mathbf{a}_1 + (2x_5 - z_5) \mathbf{a}_2 - (2x_5 + z_5 - \frac{1}{2}) \mathbf{a}_3 = -a\left(z_5 - \frac{1}{4}\right) \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{24} &= z_5 \mathbf{a}_1 - (2x_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 + (2x_5 - z_5) \mathbf{a}_3 = -a\left(z_5 - \frac{1}{4}\right) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{25} &= z_5 \mathbf{a}_1 + (2x_5 - z_5) \mathbf{a}_2 + z_5 \mathbf{a}_3 = ax_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{26} &= z_5 \mathbf{a}_1 - (2x_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3 = -a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{27} &= -\left(2x_5 + z_5 - \frac{1}{2}\right) \mathbf{a}_1 + z_5 \mathbf{a}_2 + (2x_5 - z_5) \mathbf{a}_3 = ax_5 \hat{\mathbf{x}} - a\left(z_5 - \frac{1}{4}\right) \hat{\mathbf{y}} - a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{28} &= (2x_5 - z_5) \mathbf{a}_1 + z_5 \mathbf{a}_2 - (2x_5 + z_5 - \frac{1}{2}) \mathbf{a}_3 = -a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{x}} - a\left(z_5 - \frac{1}{4}\right) \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{29} &= -z_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 + (2x_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 = a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{30} &= -z_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - (2x_5 - z_5) \mathbf{a}_3 = -ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{31} &= -(2x_5 - z_5) \mathbf{a}_1 + (2x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3 = a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a\left(z_5 + \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{32} &= (2x_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - (2x_5 - z_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 = -ax_5 \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(z_5 + \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{33} &= -(2x_5 - z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 + (2x_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 = a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{x}} + a\left(z_5 + \frac{1}{4}\right) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{34} &= (2x_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - z_5 \mathbf{a}_2 - (2x_5 - z_5) \mathbf{a}_3 = -ax_5 \hat{\mathbf{x}} + a\left(z_5 + \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{35} &= -z_5 \mathbf{a}_1 - (2x_5 - z_5) \mathbf{a}_2 - z_5 \mathbf{a}_3 = -ax_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{36} &= -z_5 \mathbf{a}_1 + (2x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3 = a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{37} &= -z_5 \mathbf{a}_1 - (2x_5 - z_5) \mathbf{a}_2 + (2x_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 = a\left(z_5 + \frac{1}{4}\right) \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{38} &= -z_5 \mathbf{a}_1 + (2x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - (2x_5 - z_5) \mathbf{a}_3 = a\left(z_5 + \frac{1}{4}\right) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{39} &= (2x_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - z_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = -az_5 \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{y}} + a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{z}} & (96g) & \text{Ge III} \\
\mathbf{B}_{40} &= -(2x_5 - z_5) \mathbf{a}_1 - z_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = -az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (96g) & \text{Ge III}
\end{aligned}$$

References

- [1] X.-J. Feng, M. Bobnar, S. Lerch, H. Biller, M. Schmidt, M. Baitinger, T. Strassner, Y. Grin, and B. Böhme, *Type-II Clathrate $\text{Na}_{24-\delta}\text{Ge}_{136}$ from a Redox-Preparation Route*, Chem. Eur. J. **27**, 12776–12787 (2021), doi:10.1002/chem.202102082.

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