

Na₄Ge₉O₂₀ Structure: A9B4C20_tI132_88_a2f_f_5f-001

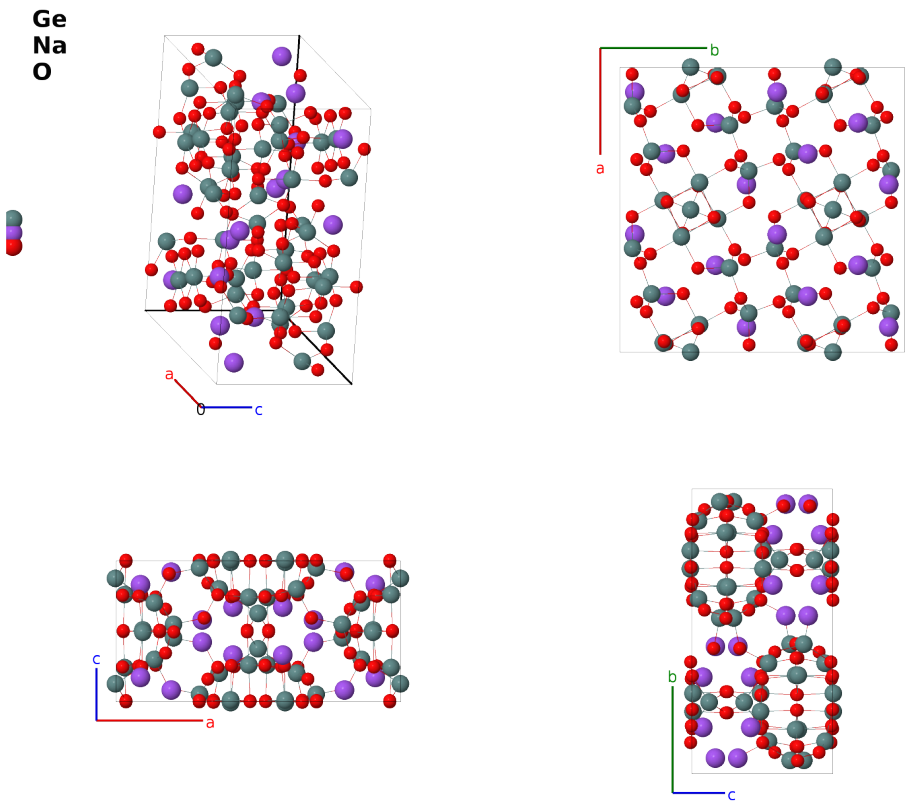
This structure previously used the label(s) **A9B4C20_tI132_88_a2f_f_5f**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/JMG5>

https://aflow.org/prototype-encyclopedia/A9B4C20_tI132_88_a2f_f_5f-001

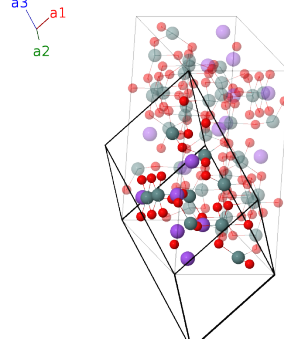


Prototype	Ge ₉ Na ₄ O ₂₀
AFLOW prototype label	A9B4C20_tI132_88_a2f_f_5f-001
ICSD	24087
CCDC	1600137
Pearson symbol	tI132
Space group number	88
Space group symbol	<i>I</i> 4 ₁ / <i>a</i>

AFLOW prototype command aflow --proto=A9B4C20_tI132_88_a2f_f_5f-001
 --params= $a, c/a, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$	(4a)	Ge I
$\mathbf{B}_2$	$= \frac{5}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$	(4a)	Ge I
$\mathbf{B}_3$	$= (y_2 + z_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_4$	$= (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - z_2) \mathbf{a}_2 - (x_2 + y_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_5$	$= (x_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - z_2) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3$	$=$	$-a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_6$	$= (-x_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 + (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_7$	$= -(y_2 + z_2) \mathbf{a}_1 - (x_2 + z_2) \mathbf{a}_2 - (x_2 + y_2) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_8$	$= (y_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 - z_2) \mathbf{a}_2 + (x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_9$	$= -(x_2 + z_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 - (x_2 - y_2) \mathbf{a}_3$	$=$	$a(y_2 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{10}$	$= (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 + (x_2 - y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Ge II
$\mathbf{B}_{11}$	$= (y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + (x_3 + y_3) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16f)	Ge III
$\mathbf{B}_{12}$	$= (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16f)	Ge III
$\mathbf{B}_{13}$	$= (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - z_3) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$	$=$	$-a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Ge III
$\mathbf{B}_{14}$	$= (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{4}) \hat{\mathbf{z}}$	(16f)	Ge III

$$\begin{aligned}
\mathbf{B}_{15} &= \begin{matrix} -(y_3 + z_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2 - \\ (x_3 + y_3) \mathbf{a}_3 \end{matrix} = -ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (16f) & \text{Ge III} \\
\mathbf{B}_{16} &= \begin{matrix} (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - z_3) \mathbf{a}_2 + (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_3 \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (16f) & \text{Ge III} \\
\mathbf{B}_{17} &= \begin{matrix} -(x_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 - z_3) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3 \end{matrix} = a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{Ge III} \\
\mathbf{B}_{18} &= \begin{matrix} (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{Ge III} \\
\mathbf{B}_{19} &= \begin{matrix} (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + \\ (x_4 + y_4) \mathbf{a}_3 \end{matrix} = ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (16f) & \text{Na I} \\
\mathbf{B}_{20} &= \begin{matrix} (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (16f) & \text{Na I} \\
\mathbf{B}_{21} &= \begin{matrix} (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_4 - z_4) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 \end{matrix} = -a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{Na I} \\
\mathbf{B}_{22} &= \begin{matrix} (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{Na I} \\
\mathbf{B}_{23} &= \begin{matrix} -(y_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 - \\ (x_4 + y_4) \mathbf{a}_3 \end{matrix} = -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (16f) & \text{Na I} \\
\mathbf{B}_{24} &= \begin{matrix} (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - z_4) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_4 \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (16f) & \text{Na I} \\
\mathbf{B}_{25} &= \begin{matrix} -(x_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_4 - z_4) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 \end{matrix} = a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{Na I} \\
\mathbf{B}_{26} &= \begin{matrix} (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{Na I} \\
\mathbf{B}_{27} &= \begin{matrix} (y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + \\ (x_5 + y_5) \mathbf{a}_3 \end{matrix} = ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{28} &= \begin{matrix} (-y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_5 - z_5) \mathbf{a}_2 - (x_5 + y_5 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_5 \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{29} &= \begin{matrix} (x_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_5 - z_5) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3 \end{matrix} = -a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{30} &= \begin{matrix} (-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{31} &= \begin{matrix} -(y_5 + z_5) \mathbf{a}_1 - (x_5 + z_5) \mathbf{a}_2 - \\ (x_5 + y_5) \mathbf{a}_3 \end{matrix} = -ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{32} &= \begin{matrix} (y_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 - z_5) \mathbf{a}_2 + (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = ax_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{33} &= \begin{matrix} -(x_5 + z_5 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_5 - z_5) \mathbf{a}_2 - (x_5 - y_5) \mathbf{a}_3 \end{matrix} = a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{34} &= \begin{matrix} (x_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} & (16f) & \text{O I} \\
\mathbf{B}_{35} &= \begin{matrix} (y_6 + z_6) \mathbf{a}_1 + (x_6 + z_6) \mathbf{a}_2 + \\ (x_6 + y_6) \mathbf{a}_3 \end{matrix} = ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16f) & \text{O II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{57} &= \begin{pmatrix} -(x_8 + z_8 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_8 - z_8) \mathbf{a}_2 - (x_8 - y_8) \mathbf{a}_3 \end{pmatrix} = a \left(y_8 - \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(x_8 - \frac{1}{4}\right) \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{4}\right) \hat{\mathbf{z}} & (16f) & \text{O IV} \\
\mathbf{B}_{58} &= \begin{pmatrix} (x_8 - z_8 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_8 + z_8 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_8 - y_8 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(y_8 - \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(x_8 + \frac{1}{4}\right) \hat{\mathbf{y}} - c \left(z_8 - \frac{1}{4}\right) \hat{\mathbf{z}} & (16f) & \text{O IV} \\
\mathbf{B}_{59} &= \begin{pmatrix} (y_9 + z_9) \mathbf{a}_1 + (x_9 + z_9) \mathbf{a}_2 + \\ (x_9 + y_9) \mathbf{a}_3 \end{pmatrix} = ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16f) & \text{O V} \\
\mathbf{B}_{60} &= \begin{pmatrix} (-y_9 + z_9 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_9 - z_9) \mathbf{a}_2 - (x_9 + y_9 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ax_9 \hat{\mathbf{x}} - a \left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16f) & \text{O V} \\
\mathbf{B}_{61} &= \begin{pmatrix} (x_9 + z_9 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_9 - z_9) \mathbf{a}_2 + (x_9 - y_9) \mathbf{a}_3 \end{pmatrix} = -a \left(y_9 + \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(x_9 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16f) & \text{O V} \\
\mathbf{B}_{62} &= \begin{pmatrix} (-x_9 + z_9 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_9 + z_9 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_9 + y_9 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(y_9 + \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(x_9 - \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{4}\right) \hat{\mathbf{z}} & (16f) & \text{O V} \\
\mathbf{B}_{63} &= \begin{pmatrix} -(y_9 + z_9) \mathbf{a}_1 - (x_9 + z_9) \mathbf{a}_2 - \\ (x_9 + y_9) \mathbf{a}_3 \end{pmatrix} = -ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16f) & \text{O V} \\
\mathbf{B}_{64} &= \begin{pmatrix} (y_9 - z_9 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_9 - z_9) \mathbf{a}_2 + (x_9 + y_9 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ax_9 \hat{\mathbf{x}} + a \left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16f) & \text{O V} \\
\mathbf{B}_{65} &= \begin{pmatrix} -(x_9 + z_9 - \frac{1}{2}) \mathbf{a}_1 + \\ (y_9 - z_9) \mathbf{a}_2 - (x_9 - y_9) \mathbf{a}_3 \end{pmatrix} = a \left(y_9 - \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(x_9 - \frac{1}{4}\right) \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{4}\right) \hat{\mathbf{z}} & (16f) & \text{O V} \\
\mathbf{B}_{66} &= \begin{pmatrix} (x_9 - z_9 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_9 + z_9 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_9 - y_9 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(y_9 - \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(x_9 + \frac{1}{4}\right) \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{4}\right) \hat{\mathbf{z}} & (16f) & \text{O V}
\end{aligned}$$

References

- [1] N. Ingri and G. Lundgren, *The Crystal Structure of $\text{Na}_4\text{Ge}_9\text{O}_{20}$* , Acta Chem. Scand. **17**, 617–633 (1963), doi:10.3891/acta.chem.scand.17-0617.

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