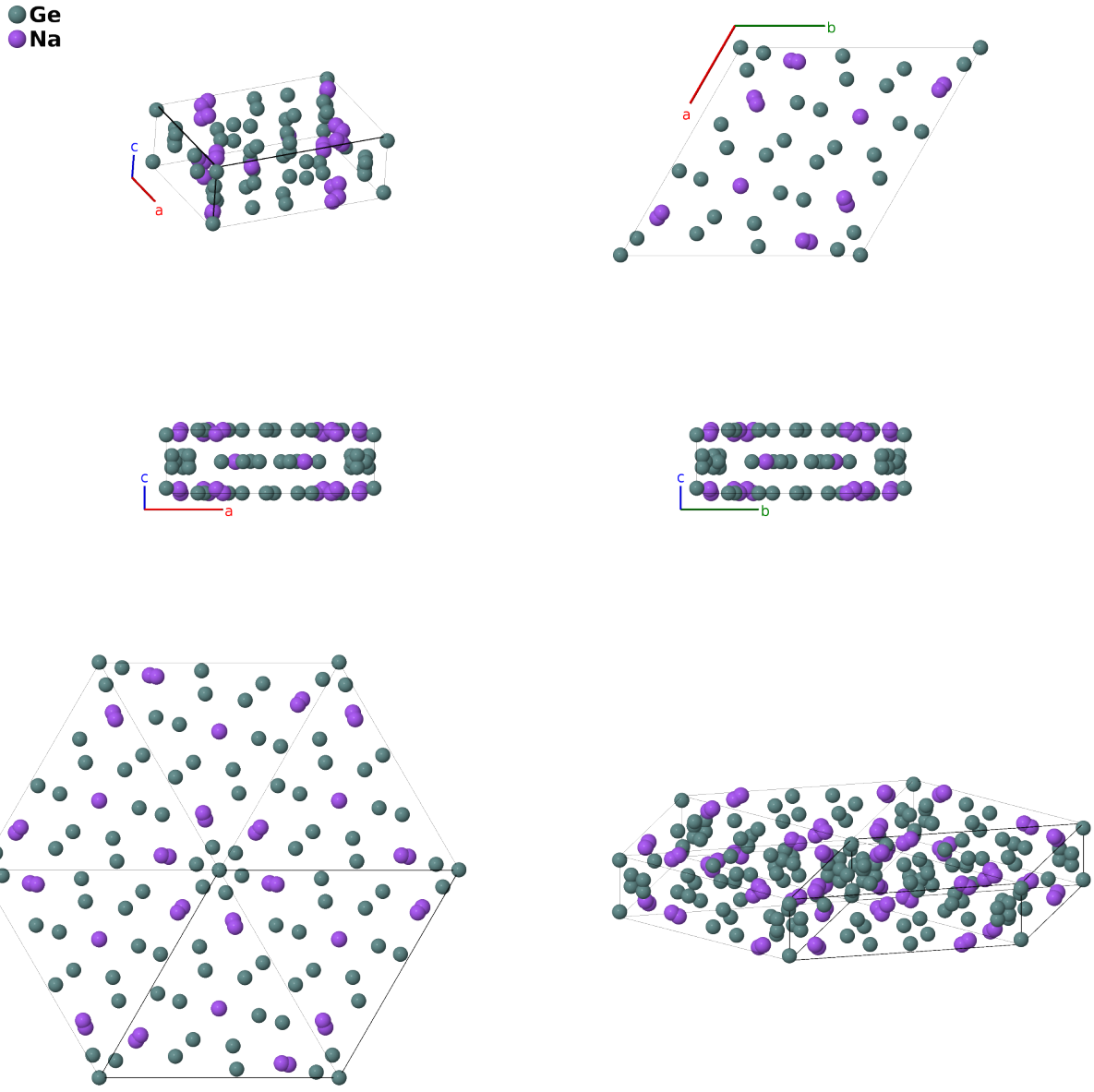
Na_4Ge_{13} Structure: A19B10_hP58_175_e2j2kl_djl-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/XPLN

https://aflow.org/p/A19B10_hP58_175_e2j2kl_djl-001



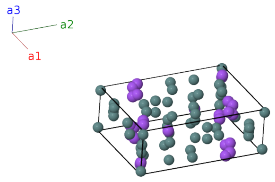
Prototype	$Ge_{13}Na_4$
AFLOW prototype label	A19B10_hP58_175_e2j2kl_djl-001
ICSD	256042
Pearson symbol	hP58

Space group number	175
Space group symbol	$P6/m$
AFLOW prototype command	`aflow --proto=A19B10_hP58_175_e2j2kl_djl-001 --params=`$a, c/a, z_2, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, z_8, x_9, y_9, z_9$

- There are a large number of vacancies in this structure leading to the composition Na_4Ge_{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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}}$	(6j)	Na II
$\mathbf{B_{18}}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(6j)	Na II
$\mathbf{B_{19}}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}$	(6j)	Na II
$\mathbf{B_{20}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$	=	$-\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}}$	(6j)	Na II

$\mathbf{B_{21}}$	$=$	$y_5\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2$	$=$	$\frac{1}{2}a\,(-x_5+2y_5)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(6j)	Na II
$\mathbf{B_{22}}$	$=$	$(x_5-y_5)\,\mathbf{a}_1+x_5\,\mathbf{a}_2$	$=$	$\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}$	(6j)	Na II
$\mathbf{B_{23}}$	$=$	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{24}}$	$=$	$-y_6\,\mathbf{a}_1+(x_6-y_6)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_6-2y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{25}}$	$=$	$-(x_6-y_6)\,\mathbf{a}_1-x_6\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{26}}$	$=$	$-x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{27}}$	$=$	$y_6\,\mathbf{a}_1-(x_6-y_6)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_6+2y_6)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{28}}$	$=$	$(x_6-y_6)\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge IV
$\mathbf{B_{29}}$	$=$	$x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7+y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_7-y_7)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge V
$\mathbf{B_{30}}$	$=$	$-y_7\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7-2y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge V
$\mathbf{B_{31}}$	$=$	$-(x_7-y_7)\,\mathbf{a}_1-x_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge V
$\mathbf{B_{32}}$	$=$	$-x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_7+y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_7-y_7)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge V
$\mathbf{B_{33}}$	$=$	$y_7\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_7+2y_7)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge V
$\mathbf{B_{34}}$	$=$	$(x_7-y_7)\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_7-y_7)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6k)	Ge V
$\mathbf{B_{35}}$	$=$	$x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{36}}$	$=$	$-y_8\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8-2y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{37}}$	$=$	$-(x_8-y_8)\,\mathbf{a}_1-x_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{38}}$	$=$	$-x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{39}}$	$=$	$y_8\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_8+2y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{40}}$	$=$	$(x_8-y_8)\,\mathbf{a}_1+x_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{41}}$	$=$	$-x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{42}}$	$=$	$y_8\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_8+2y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{43}}$	$=$	$(x_8-y_8)\,\mathbf{a}_1+x_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{44}}$	$=$	$x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8+y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_8-y_8)\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{45}}$	$=$	$-y_8\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8-2y_8)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{46}}$	$=$	$-(x_8-y_8)\,\mathbf{a}_1-x_8\,\mathbf{a}_2-z_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_8-y_8)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(12l)	Ge VI
$\mathbf{B_{47}}$	$=$	$x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{48}}$	$=$	$-y_9\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9-2y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{49}}$	$=$	$-(x_9-y_9)\,\mathbf{a}_1-x_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{50}}$	$=$	$-x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{51}}$	$=$	$y_9\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_9+2y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{52}}$	$=$	$(x_9-y_9)\,\mathbf{a}_1+x_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{53}}$	$=$	$-x_9\,\mathbf{a}_1-y_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{54}}$	$=$	$y_9\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_9+2y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{55}}$	$=$	$(x_9-y_9)\,\mathbf{a}_1+x_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{56}}$	$=$	$x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9+y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}a\,(x_9-y_9)\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{57}}$	$=$	$-y_9\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9-2y_9)\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(12l)	Na III
$\mathbf{B_{58}}$	$=$	$-(x_9-y_9)\,\mathbf{a}_1-x_9\,\mathbf{a}_2-z_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_9-y_9)\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(12l)	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* Na_4Ge_{13}, Inorg. Chem. **57**, 2002–2012 (2018), doi:10.1021/acs.inorgchem.7b02914.