

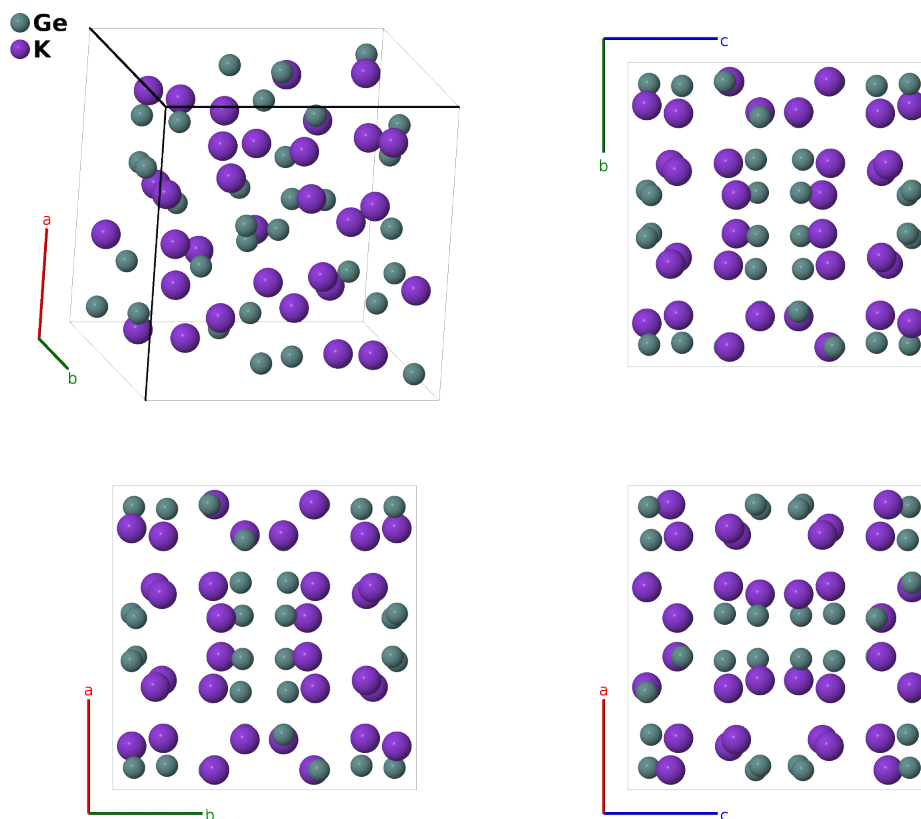
# KGe Structure:

## AB\_cP64\_218\_ei\_ei-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/RUTB>

[https://aflow.org/p/AB\\_cP64\\_218\\_ei\\_ei-001](https://aflow.org/p/AB_cP64_218_ei_ei-001)



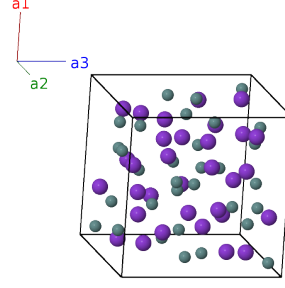
Prototype	GeK
AFLOW prototype label	AB_cP64_218_ei_ei-001
ICSD	43515
Pearson symbol	cP64
Space group number	218
Space group symbol	$P\bar{4}3n$
AFLOW prototype command	<code>aflow --proto=AB_cP64_218_ei_ei-001</code> <code>--params=<math>a, x_1, x_2, x_3, y_3, z_3, x_4, y_4, z_4</math></code>

### Other compounds with this structure

CsGe, CsSi, KSi, RbGe, RbSi

### Simple Cubic primitive vectors

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




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## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} + a x_1 \hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + a x_1 \hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} - a x_1 \hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B}_4$	$= x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} - a x_1 \hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B}_5$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B}_6$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B}_7$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B}_8$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	Ge I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} + a x_2 \hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B}_{10}$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + a x_2 \hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} - a x_2 \hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B}_{12}$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} - a x_2 \hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B}_{13}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B}_{14}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B}_{15}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B}_{16}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8e)	K I
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + a z_3 \hat{\mathbf{z}}$	(24i)	Ge II
$\mathbf{B}_{18}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} + a z_3 \hat{\mathbf{z}}$	(24i)	Ge II
$\mathbf{B}_{19}$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} - a z_3 \hat{\mathbf{z}}$	(24i)	Ge II
$\mathbf{B}_{20}$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} - a z_3 \hat{\mathbf{z}}$	(24i)	Ge II
$\mathbf{B}_{21}$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$a z_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + a y_3 \hat{\mathbf{z}}$	(24i)	Ge II
$\mathbf{B}_{22}$	$= z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$a z_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - a y_3 \hat{\mathbf{z}}$	(24i)	Ge II
$\mathbf{B}_{23}$	$= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-a z_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + a y_3 \hat{\mathbf{z}}$	(24i)	Ge II
$\mathbf{B}_{24}$	$= -z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$-a z_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} - a y_3 \hat{\mathbf{z}}$	(24i)	Ge II



$$\begin{aligned}
\mathbf{B}_{55} &= \begin{pmatrix} (y_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 - \\ (z_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left( y_4 + \frac{1}{2} \right) \hat{\mathbf{x}} - a \left( x_4 - \frac{1}{2} \right) \hat{\mathbf{y}} - a \left( z_4 - \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II} \\
\mathbf{B}_{56} &= - \begin{pmatrix} (y_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 - \\ (z_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left( y_4 - \frac{1}{2} \right) \hat{\mathbf{x}} + a \left( x_4 + \frac{1}{2} \right) \hat{\mathbf{y}} - a \left( z_4 - \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II} \\
\mathbf{B}_{57} &= \begin{pmatrix} (x_4 + \frac{1}{2}) \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left( x_4 + \frac{1}{2} \right) \hat{\mathbf{x}} + a \left( z_4 + \frac{1}{2} \right) \hat{\mathbf{y}} + a \left( y_4 + \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II} \\
\mathbf{B}_{58} &= - \begin{pmatrix} (x_4 - \frac{1}{2}) \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 - \\ (y_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left( x_4 - \frac{1}{2} \right) \hat{\mathbf{x}} + a \left( z_4 + \frac{1}{2} \right) \hat{\mathbf{y}} - a \left( y_4 - \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II} \\
\mathbf{B}_{59} &= - \begin{pmatrix} (x_4 - \frac{1}{2}) \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 + \\ (y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left( x_4 - \frac{1}{2} \right) \hat{\mathbf{x}} - a \left( z_4 - \frac{1}{2} \right) \hat{\mathbf{y}} + a \left( y_4 + \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II} \\
\mathbf{B}_{60} &= \begin{pmatrix} (x_4 + \frac{1}{2}) \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 - \\ (y_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left( x_4 + \frac{1}{2} \right) \hat{\mathbf{x}} - a \left( z_4 - \frac{1}{2} \right) \hat{\mathbf{y}} - a \left( y_4 - \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II} \\
\mathbf{B}_{61} &= \begin{pmatrix} (z_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left( z_4 + \frac{1}{2} \right) \hat{\mathbf{x}} + a \left( y_4 + \frac{1}{2} \right) \hat{\mathbf{y}} + a \left( x_4 + \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II} \\
\mathbf{B}_{62} &= \begin{pmatrix} (z_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - \\ (x_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left( z_4 + \frac{1}{2} \right) \hat{\mathbf{x}} - a \left( y_4 - \frac{1}{2} \right) \hat{\mathbf{y}} - a \left( x_4 - \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II} \\
\mathbf{B}_{63} &= - \begin{pmatrix} (z_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - \\ (x_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left( z_4 - \frac{1}{2} \right) \hat{\mathbf{x}} + a \left( y_4 + \frac{1}{2} \right) \hat{\mathbf{y}} - a \left( x_4 - \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II} \\
\mathbf{B}_{64} &= - \begin{pmatrix} (z_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left( z_4 - \frac{1}{2} \right) \hat{\mathbf{x}} - a \left( y_4 - \frac{1}{2} \right) \hat{\mathbf{y}} + a \left( x_4 + \frac{1}{2} \right) \hat{\mathbf{z}} & (24i) & \text{K II}
\end{aligned}$$

## References

- [1] E. Busmann, *Das Verhalten der Alkalimetalle zu Halbmetallen. X. Die Kristallstrukturen von KSi, RbSi, CsSi, KGe, RbGe und CsGe*, Z. Anorganische und Allgemeine Chemie **313**, 90–106 (1961), doi:10.1002/zaac.19613130108.

## Found in

- [1] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2, International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).