

K₂GeF₆ (J1₁₃) Structure: A6BC2_hP9_164_i_a_d-001

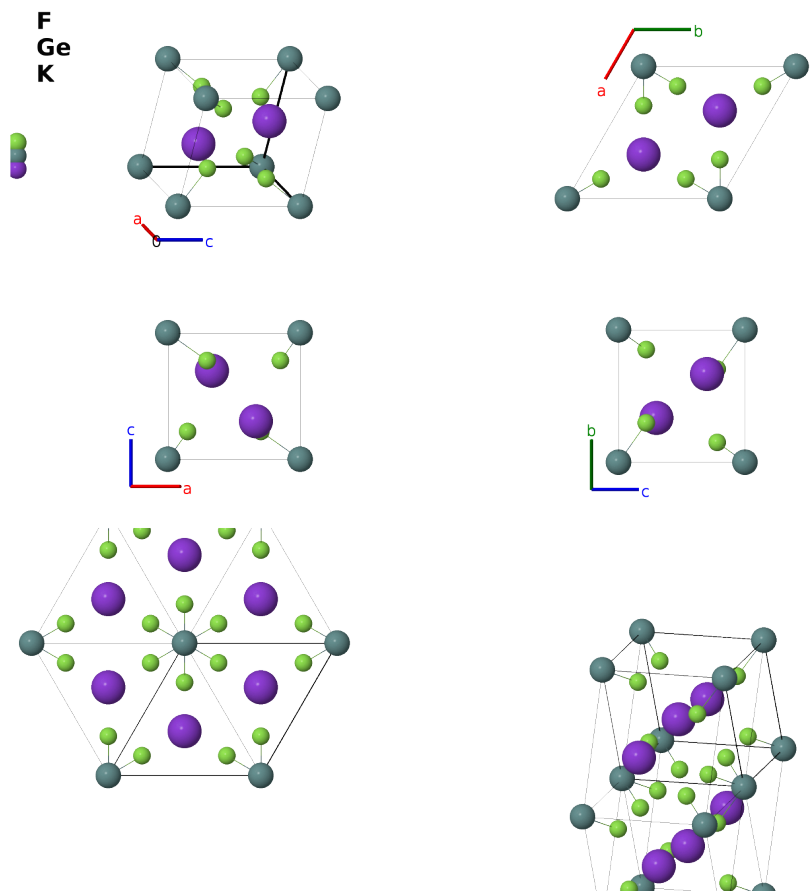
This structure previously used the label(s) **A6BC2_hP9_164_i_a_d**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/2HX1>

https://aflow.org/prototype-encyclopedia/A6BC2_hP9_164_i_a_d-001



Prototype	F ₆ GeK ₂
AFLOW prototype label	A6BC2_hP9_164_i_a_d-001
Strukturbericht designation	J1 ₁₃
ICSD	24026
CCDC	1600082
Pearson symbol	hP9
Space group number	164

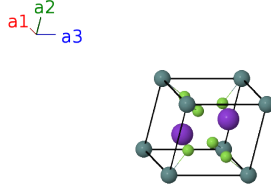
Space group symbol $P\bar{3}m1$

AFLOW prototype command `aflow --proto=A6BC2_hP9_164_i_a_d-001`
`--params=a, c/a, z2, x3, z3`

Other compounds with this structure

(NH₄)₂GeF₆, Cs₂CeCl₆, K₂PtF₆, K₂SiF₆

Trigonal (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
$\mathbf{B}_1$	=	0	=	0	(1a) Ge I
$\mathbf{B}_2$	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2d) K I
$\mathbf{B}_3$	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2d) K I
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-\sqrt{3}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6i) F I
$\mathbf{B}_5$	=	$x_3 \mathbf{a}_1 + 2x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6i) F I
$\mathbf{B}_6$	=	$-2x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6i) F I
$\mathbf{B}_7$	=	$-x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$\sqrt{3}ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6i) F I
$\mathbf{B}_8$	=	$2x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6i) F I
$\mathbf{B}_9$	=	$-x_3 \mathbf{a}_1 - 2x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-\frac{3}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6i) F I

References

- [1] J. L. Hoard and W. B. Vincent, *Structures of Complex Fluorides. Potassium Hexafluogermanate and Ammonium Hexafluogermanate*, J. Am. Chem. Soc. **61**, 2849–2852 (1939), doi:10.1021/ja01265a082.

Found in

- [1] T. Kaatz and M. Marcovich, *The crystal structure of the compound Cs₂CeCl₆*, Acta Cryst. **21**, 1011 (1966), doi:10.1107/S0365110X66004419.

First cited in

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