K_2GeF_6 ($J1_{13}$) Structure: A6BC2_hP9_164_i_a_d-001

This structure originally had the label `A6BC2_hP9_164_i_a_d`. Calls to that address will be redirected here.

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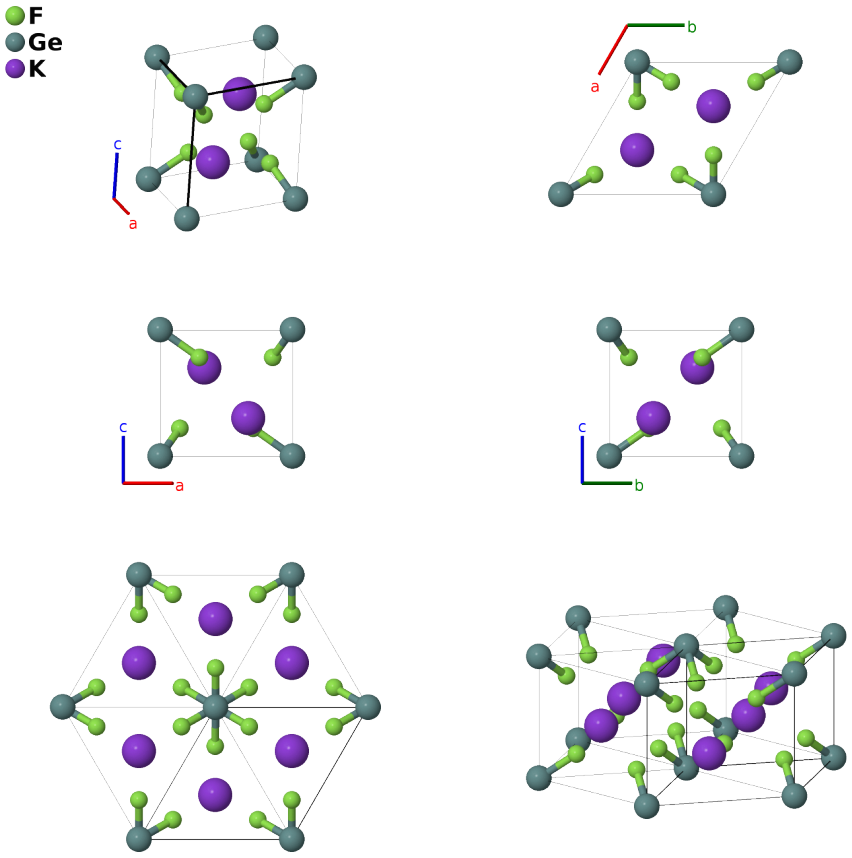
https://aflow.org/p/2HX1

https://aflow.org/p/A6BC2_hP9_164_i_a_d-001

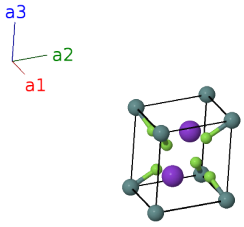


Prototype	F_6GeK_2
AFLOW prototype label	A6BC2_hP9_164_i_a_d-001
***Strukturbericht* designation**	$J1_{13}$
ICSD	24026
Pearson symbol	hP9
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=A6BC2_hP9_164_i_a_d-001 --params=`$a, c/a, z_2, x_3, z_3$

Other compounds with this structure
$(NH_4)_2GeF_6$, Cs_2CeCl_6, K_2PtF_6, K_2SiF_6

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



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 Cs_2CeCl_6*, Acta Cryst. **21**, 1011 (1966), doi:10.1107/S0365110X66004419.