β_1-K_2UF_6 Structure: A6B2C_hP9_189_fg_c_b-001

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https://aflow.org/p/XTDJ

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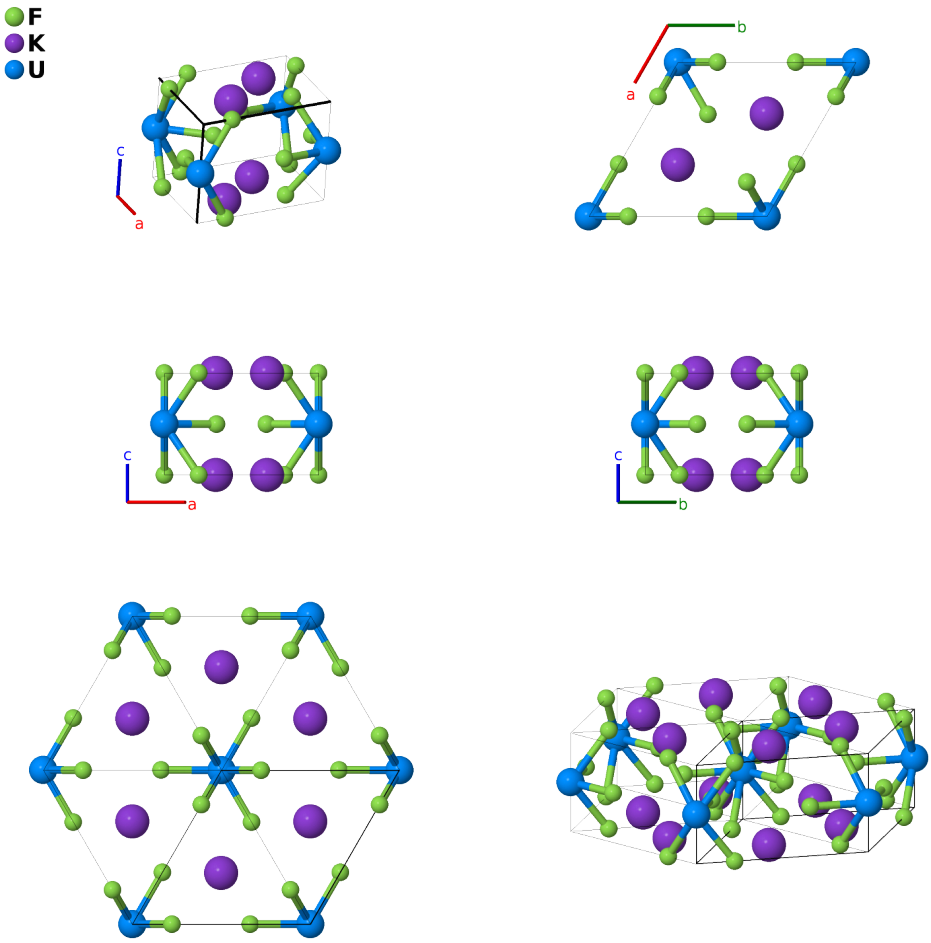


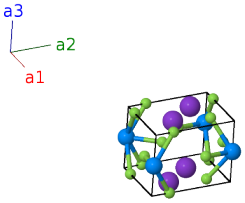
Prototype	F_6K_2U
AFLOW prototype label	A6B2C_hP9_189_fg_c_b-001
ICSD	26193
Pearson symbol	hP9
Space group number	189
Space group symbol	$P\bar{6}2m$
AFLOW prototype command	`aflow --proto=A6B2C_hP9_189_fg_c_b-001 --params=`$a, c/a, x_3, x_4$

Other compounds with this structure
K_2CeF_6, K_2ThF_6, δ-Na_2UF_6

- α-K_2UF_6 is in the cubic fluorite ($C1$, CaF_2) structure, with the potassium and uranium atoms placed randomly on the calcium sites.
- β_2-K_2UF_6 takes on the trigonal β-Na_2ThF_6 structure.

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
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	U I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	K I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	K I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	F I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	F I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(3f)	F I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	F II
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	F II
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	F II

References

[1] G. Brunton, *Refinement of the crystal structure of β_1-K_2UF_6*, Acta Crystallogr. Sect. B **25**, 2163–2164 (1969), doi:10.1107/S0567740869005310.

Found in

[1] A. Grzechnik, C. C. Underwood, J. W. Kolis, and K. Friese, *Crystal structures and stability of K_2ThF_6 and $K_7Th_6F_{31}$ on compression*, J. Fluor. Chem. **150**, 8–13 (2013), doi:10.1016/j.jfluchem.2013.02.024.