

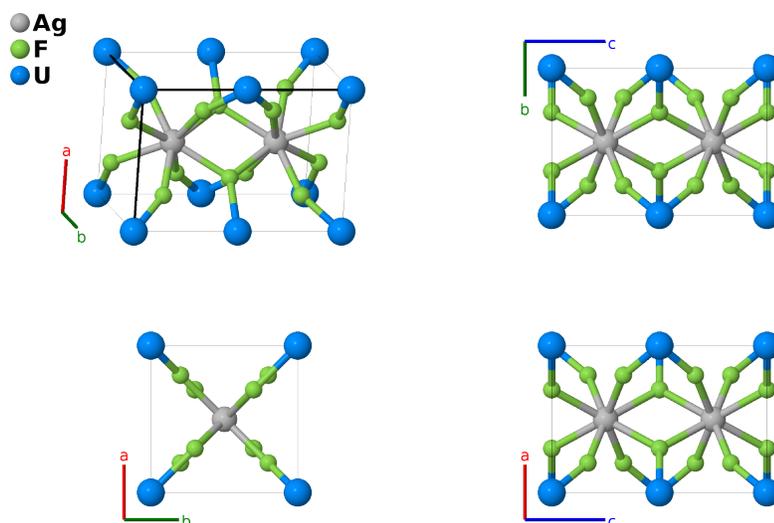
AgUF₆ Structure: AB6C_tP16_132_b_io_c-001

This structure originally had the label AB6C_tP16_132_d_io_a. Calls to that address will be redirected here.

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<https://aflow.org/p/U3ZM>

https://aflow.org/p/AB6C_tP16_132_b_io_c-001

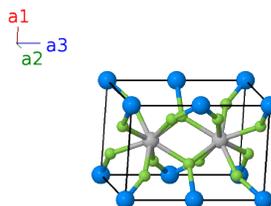


Prototype	AgF ₆ U
AFLOW prototype label	AB6C_tP16_132_b_io_c-001
ICSD	none
Pearson symbol	tP16
Space group number	132
Space group symbol	<i>P4</i> ₂ / <i>mcm</i>
AFLOW prototype command	<code>aflow --proto=AB6C_tP16_132_b_io_c-001 --params=a, c/a, x₃, x₄, z₄</code>

Other compounds with this structure
RbUF₆, TlUF₆, (NH₄)UF₆

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Ag I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_3$	=	$\frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Ag I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(2c)	U I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2c)	U I
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	=	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(4i)	F I
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	=	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(4i)	F I
\mathbf{B}_7	$= -x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4i)	F I
\mathbf{B}_8	$= x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4i)	F I
\mathbf{B}_9	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8o)	F II
\mathbf{B}_{10}	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8o)	F II
\mathbf{B}_{11}	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8o)	F II
\mathbf{B}_{12}	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8o)	F II
\mathbf{B}_{13}	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8o)	F II
\mathbf{B}_{14}	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8o)	F II
\mathbf{B}_{15}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8o)	F II
\mathbf{B}_{16}	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8o)	F II

References

- [1] P. Charpin, *Structure cristalline des hexafluorures complexes d'uranium V et d'argent, de potassium, d'ammonium, de rubidium ou de thallium*, C. R. Hebd. Séances Acad. Sci. **260**, 1914–1916 (1965).

Found in

- [1] P. Villars, *AgUF6 Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database).