

AgUF₆ Structure: AB6C_tP16_132_b_io_c-001

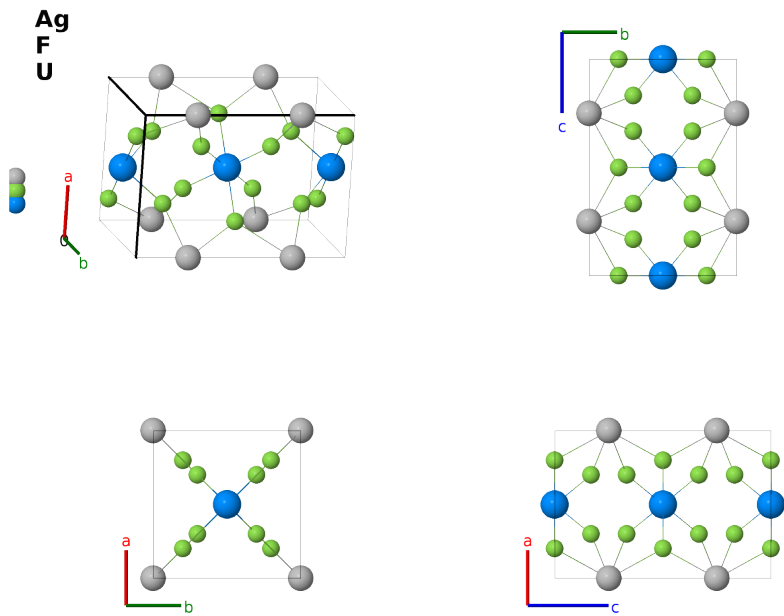
This structure previously used the label(s) **AB6C_tP16_132_d_io_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/U3ZM>

https://aflow.org/prototype-encyclopedia/AB6C_tP16_132_b_io_c-001



Prototype	AgF ₆ U
AFLOW prototype label	AB6C_tP16_132_b_io_c-001
Pearson symbol	tP16
Space group number	132
Space group symbol	$P4_2/mcm$
AFLOW prototype command	<code>aflow --proto=AB6C_tP16_132_b_io_c-001</code> <code>--params=a, c/a, x₃, x₄, z₄</code>

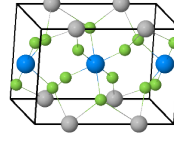
Other compounds with this structure

RbUF₆, TiUF₆, (NH₄)UF₆

Simple Tetragonal primitive vectors

a1
a2
a3

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8o)	F II
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8o)	F II
$\mathbf{B}_{13}$	$= -x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8o)	F II
$\mathbf{B}_{14}$	$= x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(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).

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- D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043