AuF$_3$ Structure: AB3_hP24_179_b_ac-001
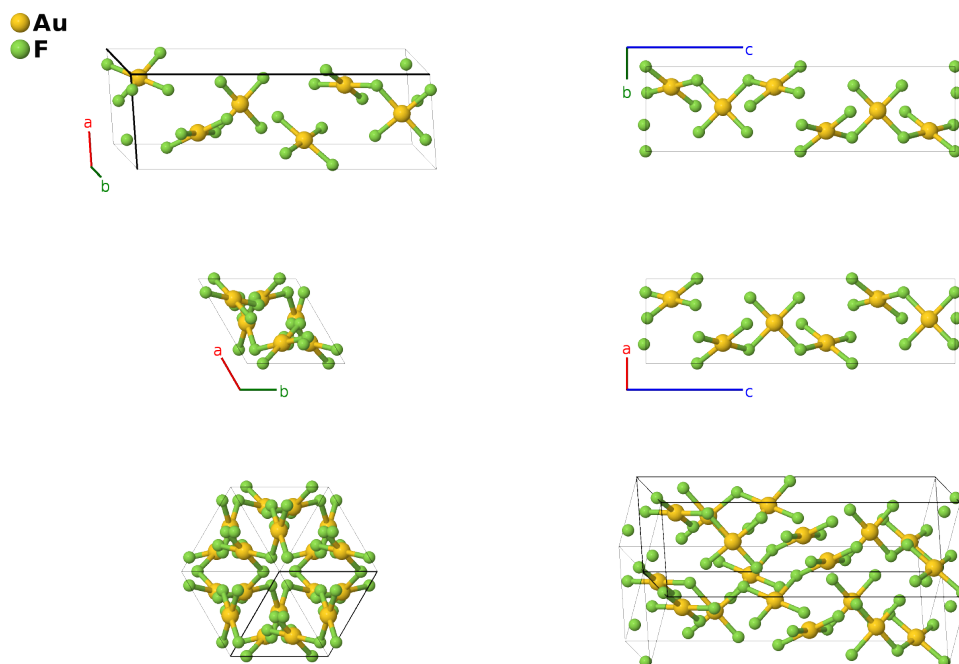
This structure originally had the label `AB3_hP24_179_b_ac`. Calls to that address will be redirected here.

https://aflow.org/p/45S0

https://aflow.org/p/AB3_hP24_179_b_ac-001

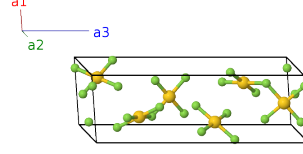|	
Prototype	AuF$_3$
AFLOW prototype label	AB3_hP24_179_b_ac-001
ICSD	none
Pearson symbol	hP24
Space group number	179
Space group symbol	$P6_522$
AFLOW prototype command	aflow --proto=AB3_hP24_179_b_ac-001 --params=$a, c/a, x_1, x_2, x_3, y_3, z_3$

Other compounds with this structure

AgF$_3$

- These compounds also exist in the enantiomorphic space group $P6_122$ #178. That page describes the more recent (Žemva, 1991) determination of the structure.

Hexagonal primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1}$	$=$	$\tfrac{1}{2}ax_1\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(6a)	F I
$\mathbf{B_2}$	$=$	$x_1\,\mathbf{a_2} + \tfrac{2}{3}\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}ax_1\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \tfrac{2}{3}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a_1} - x_1\,\mathbf{a_2} + \tfrac{1}{3}\,\mathbf{a_3}$	$=$	$-ax_1\,\hat{\mathbf{x}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_4}$	$=$	$-x_1\,\mathbf{a_1} + \tfrac{1}{2}\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}ax_1\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_5}$	$=$	$-x_1\,\mathbf{a_2} + \tfrac{1}{6}\,\mathbf{a_3}$	$=$	$-\tfrac{1}{2}ax_1\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \tfrac{1}{6}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_6}$	$=$	$x_1\,\mathbf{a_1} + x_1\,\mathbf{a_2} + \tfrac{5}{6}\,\mathbf{a_3}$	$=$	$ax_1\,\hat{\mathbf{x}} + \tfrac{5}{6}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_7}$	$=$	$x_2\,\mathbf{a_1} + 2x_2\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_2\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \tfrac{3}{4}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_8}$	$=$	$-2x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} + \tfrac{5}{12}\,\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_2\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \tfrac{5}{12}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_9}$	$=$	$x_2\,\mathbf{a_1} - x_2\,\mathbf{a_2} + \tfrac{1}{12}\,\mathbf{a_3}$	$=$	$-\sqrt{3}ax_2\,\hat{\mathbf{y}} + \tfrac{1}{12}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_{10}}$	$=$	$-x_2\,\mathbf{a_1} - 2x_2\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	$=$	$-\tfrac{3}{2}ax_2\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \tfrac{1}{4}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_{11}}$	$=$	$2x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + \tfrac{11}{12}\,\mathbf{a_3}$	$=$	$\tfrac{3}{2}ax_2\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \tfrac{11}{12}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_{12}}$	$=$	$-x_2\,\mathbf{a_1} + x_2\,\mathbf{a_2} + \tfrac{7}{12}\,\mathbf{a_3}$	$=$	$\sqrt{3}ax_2\,\hat{\mathbf{y}} + \tfrac{7}{12}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_{13}}$	$=$	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{14}}$	$=$	$-y_3\,\mathbf{a_1} + \left(x_3 - y_3\right)\mathbf{a_2} + \left(z_3 + \tfrac{2}{3}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 - 2y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \tfrac{1}{3}c\left(3z_3 + 2\right)\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{15}}$	$=$	$-\left(x_3 - y_3\right)\mathbf{a_1} - x_3\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{3}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{3}\right)\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{16}}$	$=$	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{17}}$	$=$	$y_3\,\mathbf{a_1} - \left(x_3 - y_3\right)\mathbf{a_2} + \left(z_3 + \tfrac{1}{6}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_3 + 2y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{6}\right)\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{18}}$	$=$	$\left(x_3 - y_3\right)\mathbf{a_1} + x_3\,\mathbf{a_2} + \left(z_3 + \tfrac{5}{6}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \tfrac{1}{6}c\left(6z_3 + 5\right)\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{19}}$	$=$	$y_3\,\mathbf{a_1} + x_3\,\mathbf{a_2} - \left(z_3 - \tfrac{2}{3}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} - \tfrac{1}{3}c\left(3z_3 - 2\right)\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{20}}$	$=$	$\left(x_3 - y_3\right)\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(x_3 - 2y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{21}}$	$=$	$-x_3\,\mathbf{a_1} - \left(x_3 - y_3\right)\mathbf{a_2} - \left(z_3 - \tfrac{1}{3}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{3}\right)\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{22}}$	$=$	$-y_3\,\mathbf{a_1} - x_3\,\mathbf{a_2} - \left(z_3 - \tfrac{1}{6}\right)\mathbf{a_3}$	$=$	$-\tfrac{1}{2}a\left(x_3 + y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{6}\right)\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{23}}$	$=$	$-\left(x_3 - y_3\right)\mathbf{a_1} + y_3\,\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(-x_3 + 2y_3\right)\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{24}}$	$=$	$x_3\,\mathbf{a_1} + \left(x_3 - y_3\right)\mathbf{a_2} - \left(z_3 - \tfrac{5}{6}\right)\mathbf{a_3}$	$=$	$\tfrac{1}{2}a\left(2x_3 - y_3\right)\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - \tfrac{1}{6}c\left(6z_3 - 5\right)\hat{\mathbf{z}}$	(12c)	F II

References

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[2] B. Žemva, K. Lutar, A. Jesih, W. J. C. Jr., A. P. Wilkinson, D. E. Cox, R. B. V. Dreele, H. Borrmann, and N. Bartlett, *Silver trifluoride: preparation, crystal structure, some properties, and comparison with AuF_3*, J. Am. Chem. Soc. **113**, 4192–4198 (1991), doi:10.1021/ja00011a021.

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