AuF_3 Structure: AB3_hP24_178_b_ac-001

This structure originally had the label `AB3_hP24_178_b_ac`. Calls to that address will be redirected here.

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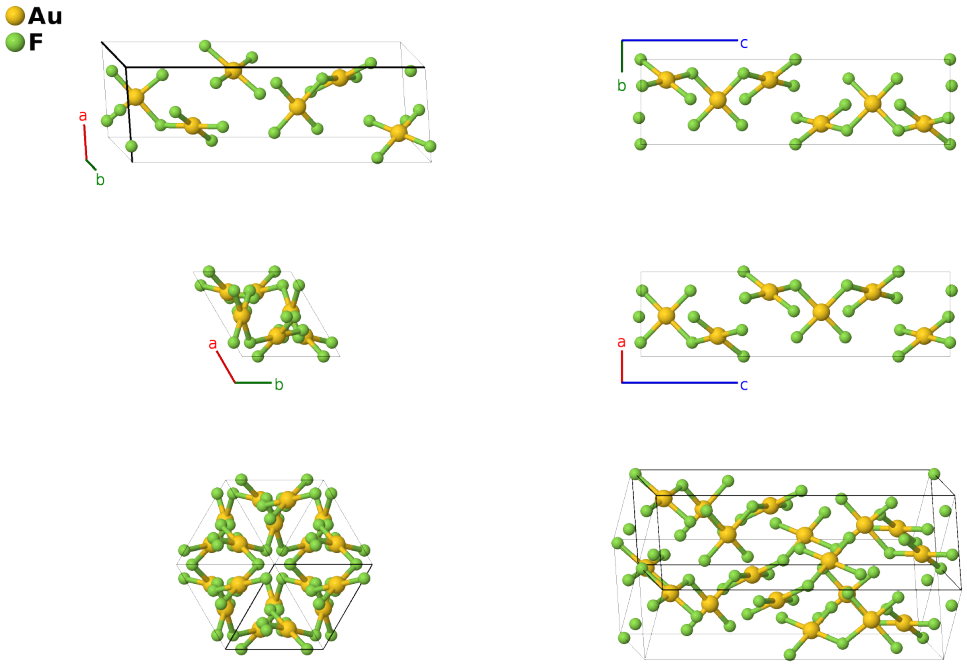
https://aflow.org/p/UBNE

https://aflow.org/p/AB3_hP24_178_b_ac-001



Prototype	AuF_3
AFLOW prototype label	AB3_hP24_178_b_ac-001
ICSD	80478
Pearson symbol	hP24
Space group number	178
Space group symbol	$P6_122$
AFLOW prototype command	`aflow --proto=AB3_hP24_178_b_ac-001 --params=`$a, c/a, x_1, x_2, x_3, y_3, z_3$

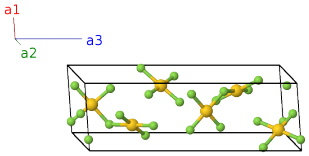
Other compounds with this structure
AgF_3

- Previously (Hicks, 2019) used the data from (Asprey, 1964) to describe this structure. We have updated this to use the more recent data from (Žemva, 1991). This does not change the essential nature of the structure.

- This structure can also be found in the enantiomorphic space group $P6_522$ #179. That page presents the original data from (Asprey, 1964).

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}}$	(6a)	F I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{5}{6}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_6}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \frac{1}{6}\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(6a)	F I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_8}$	=	$-2x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{7}{12}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{7}{12}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{11}{12}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{11}{12}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_{10}}$	=	$-x_2\,\mathbf{a}_1 - 2x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_{11}}$	=	$2x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{12}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{12}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_{12}}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{5}{12}\,\mathbf{a}_3$	=	$\sqrt{3}ax_2\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6b)	Au I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{14}}$	=	$-y_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{15}}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3 + \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3 + 2)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{16}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{17}}$	=	$y_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{5}{6}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3 + 2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{6}c\,(6z_3 + 5)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{18}}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{6}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{6}\right)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{19}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{20}}$	=	$(x_3 - y_3)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{21}}$	=	$-x_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_3 - 2)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{22}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3 - \frac{5}{6}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} - \frac{1}{6}c\,(6z_3 - 5)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{23}}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3 + 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{24}}$	=	$x_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{6}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{6}\right)\,\hat{\mathbf{z}}$	(12c)	F II

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[3] L. B. Asprey, F. H. Kruse, K. H. Jack, and R. Maitland, *Preparation and Properties of Crystalline Gold Trifluoride*, Inorg. Chem. **3**, 602–604 (1964), doi:10.1021/ic50014a037.

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