AuF_3 Structure: AB3_hP24_179_b_ac-001

This structure previously used the label(s) `AB3_hP24_179_b_ac`. Calls to these addresses will be redirected here.

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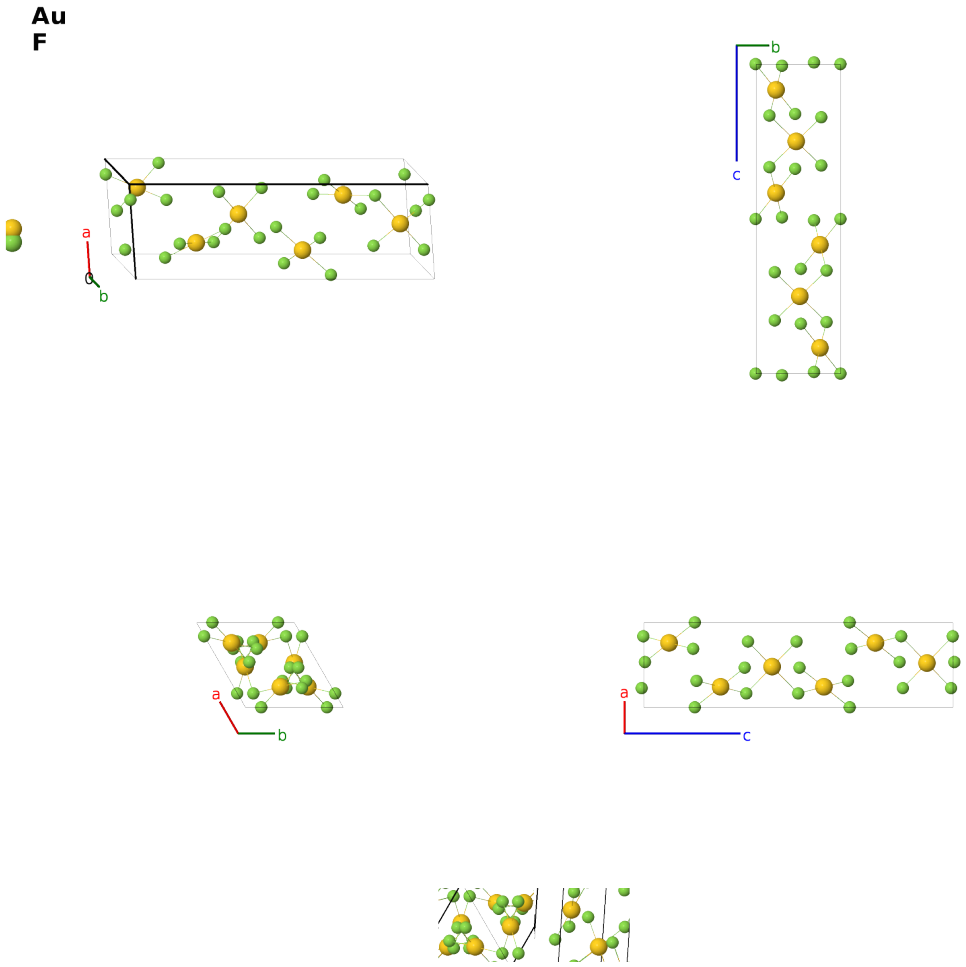
https://aflow.org/prototype-encyclopedia/45S0

https://aflow.org/prototype-encyclopedia/AB3_hP24_179_b_ac-001



Prototype	AuF_3
AFLOW prototype label	AB3_hP24_179_b_ac-001
Pearson symbol	hP24
Space group number	179
Space group symbol	$P6_522$

AFLOW prototype command `aflow --proto=AB3_hP24_179_b_ac-001 --params=`$a, c/a, x_1, x_2, x_3, y_3, z_3$

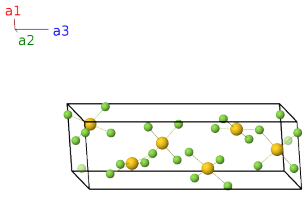
Other compounds with this structure

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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



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

$\mathbf{B_{19}}$	$=$	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(z_3 - \frac{2}{3}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_3 - 2)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{21}}$	$=$	$-x_3\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{3}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B_{22}}$	$=$	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{6}\right)\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{6}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{24}}$	$=$	$x_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{5}{6}\right)\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - \frac{1}{6}c\,(6z_3 - 5)\,\hat{\mathbf{z}}$	(12c)	F II

References

[1] 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.

[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.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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