

AuF₃ Structure:

AB3_hP24_178_b_ac-001

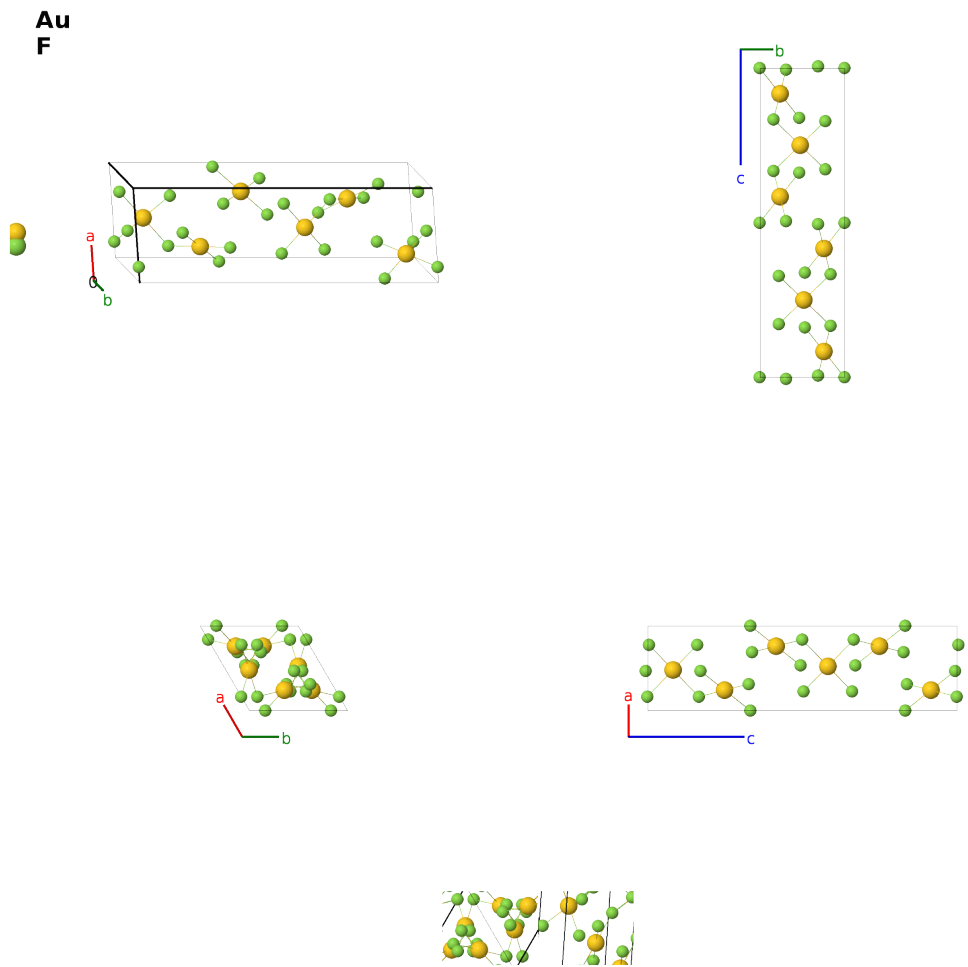
This structure previously used the label(s) **AB3_hP24_178.b.ac**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/AB3_hP24_178_b_ac-001



Prototype	AuF ₃
AFLOW prototype label	AB3_hP24_178_b_ac-001
ICSD	80478
CCDC	1640686
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, x1, x2, x3, y3, z3`

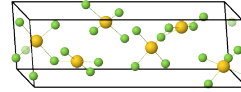
Other compounds with this structure

AgF₃

- 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B}_{14}$	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(12c)	F II
$\mathbf{B}_{15}$	$-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	=	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(12c)	F II

$$\begin{aligned}
\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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{F II}
\end{aligned}$$

References

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- [2] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.
- [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.

Found in

- [1] P. Villars, *AuF₃ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

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