

AgF₂ Structure:

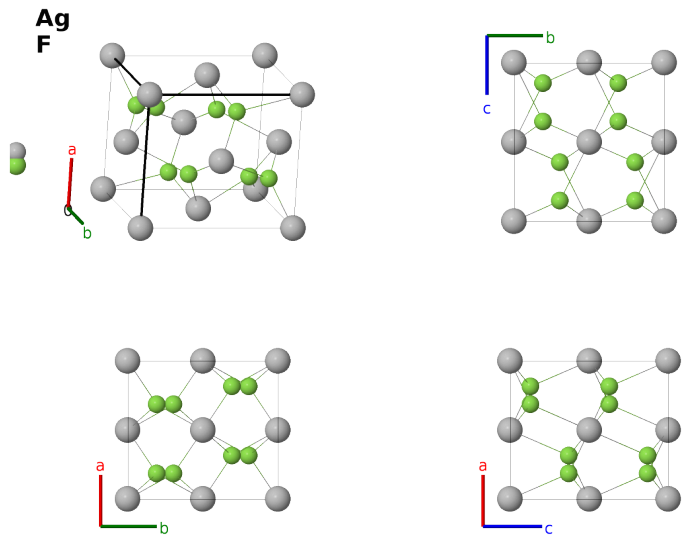
AB2_oP12_61_a_c-002

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<https://aflow.org/prototype-encyclopedia/F3J5>

https://aflow.org/prototype-encyclopedia/AB2_oP12_61_a_c-002

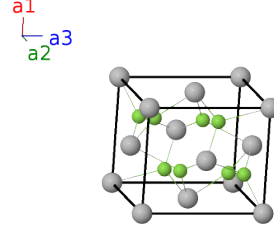


Prototype	AgF ₂
AFLOW prototype label	AB2_oP12_61_a_c-002
ICSD	9922
CCDC	1594813
Pearson symbol	oP12
Space group number	61
Space group symbol	<i>Pbca</i>
AFLOW prototype command	<code>aflow --proto=AB2_oP12_61_a_c-002</code> <code>--params=a, b/a, c/a, x₂, y₂, z₂</code>

- This is a distortion of the fluorite (*C1*) structure. We can recover that structure when $a = b = c$ and $x_2 = y_2 = z_2 = 1/2$.
- β -HgO₂, AgF₂, and PdSe₂ have the same AFLOW prototype label, AB2_oP12_61_a_c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(4a) Ag I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a) Ag I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a) Ag I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(4a) Ag I
$\mathbf{B}_5$	$=$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c) F I
$\mathbf{B}_6$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c) F I
$\mathbf{B}_7$	$=$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c) F I
$\mathbf{B}_8$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c) F I
$\mathbf{B}_9$	$=$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c) F I
$\mathbf{B}_{10}$	$=$	$(x_2 + \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c) F I
$\mathbf{B}_{11}$	$=$	$x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c) F I
$\mathbf{B}_{12}$	$=$	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c) F I

References

- [1] P. Fischer, D. Schwarzenbach, and H. M. Rietveld, *Crystal and magnetic structure of silver difluoride: I. Determination of the AgF_2 structure*, J. Phys. Chem. Solids **32**, 543–550 (1971), doi:10.1016/0022-3697(71)90003-5.

Found in

- [1] P. Fischer, G. Roult, and D. Schwarzenbach, *Crystal and magnetic structure of silver difluoride-II. Weak 4d-ferromagnetism of AgF_2* , J. Phys. Chem. Solids **32**, 1641–1647 (1971), doi:10.1016/S0022-3697(71)80057-4.

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