

BaZnF₄ Structure:

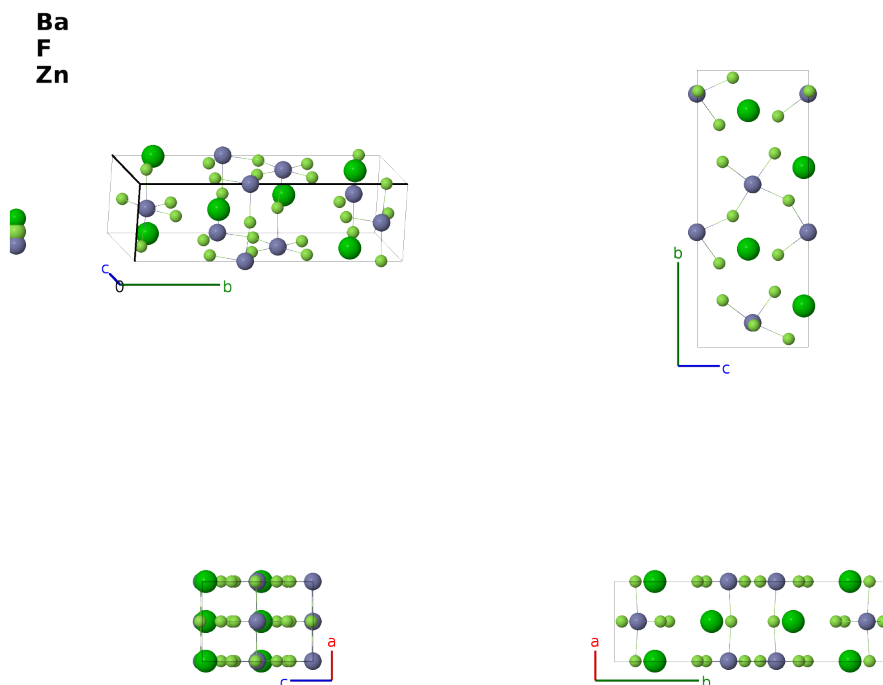
AB4C_oC24_36_a_4a_a-002

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<https://aflow.org/prototype-encyclopedia/F77P>

https://aflow.org/prototype-encyclopedia/AB4C_oC24_36_a_4a_a-002



Prototype	BaF ₄ Zn
AFLOW prototype label	AB4C_oC24_36_a_4a_a-002
ICSD	402925
CCDC	1724960
Pearson symbol	oC24
Space group number	36
Space group symbol	<i>Cmc</i> 2 ₁
AFLOW prototype command	<pre>aflow --proto=AB4C_oC24_36_a_4a_a-002 --params=a,b/a,c/a,y1,z1,y2,z2,y3,z3,y4,z4,y5,z5,y6,z6</pre>

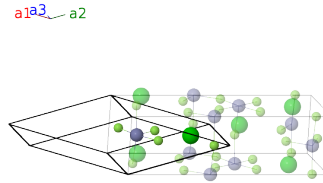
Other compounds with this structure

BaCoF₄, BaCuF₄, BaFeF₄, BaMgF₄, BaMnF₄, BaNiF₄, BaWO₄, BiNbO₄, EuMgD₄, HfGeTe₄, LaTaO₄, NaAlH₄, NaOsO₄, SrMgD₄, SrMgF₄, ZrGeTe₄

- While many of the listed compounds have a phase transition under pressure they do not necessarily transform into the same structure.
 - Above 5 GPa BaZnF₄ transforms into its high pressure structure. (Posse, 2011)
 - We use the data from (Lapasset, 1996) taken at 295K.
 - Space group $Cmc2_1$ #36 allows an arbitrary choice of the origin of the z -axis. Here we set $z_6 = 0$ for the zinc (2a) site.
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Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Ba I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Ba I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	F I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	F I
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	F II
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	F II
$\mathbf{B}_7$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	F III
$\mathbf{B}_8$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	F III
$\mathbf{B}_9$	$= -y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4a)	F IV
$\mathbf{B}_{10}$	$= y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	F IV
$\mathbf{B}_{11}$	$= -y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4a)	Zn I
$\mathbf{B}_{12}$	$= y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} + c \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Zn I

References

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Found in

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First cited in

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