

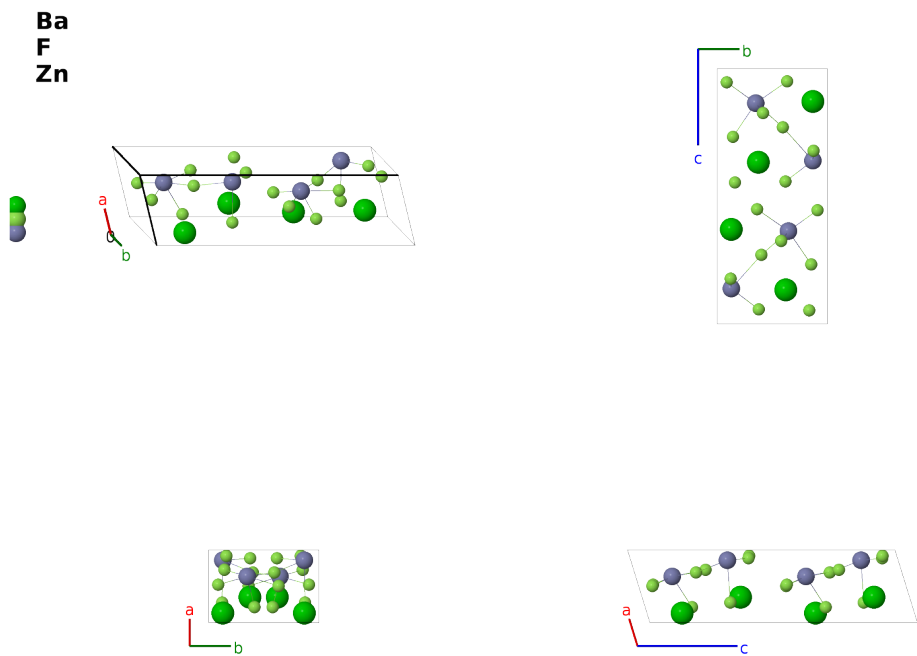
High Pressure BaZnF₄ Structure: AB4C_mP24_7_2a_8a_2a-001

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<https://aflow.org/prototype-encyclopedia/0MGD>

https://aflow.org/prototype-encyclopedia/AB4C_mP24_7_2a_8a_2a-001

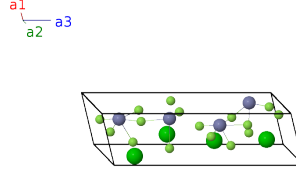


Prototype	BaF ₄ Zn
AFLOW prototype label	AB4C_mP24_7_2a_8a_2a-001
ICSD	182608
CCDC	1783367
Pearson symbol	mP24
Space group number	7
Space group symbol	<i>Pc</i>
AFLOW prototype command	<pre>aflow --proto=AB4C_mP24_7_2a_8a_2a-001 --params=a,b/a,c/a,β,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇, y₇,z₇,x₈,y₈,z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂</pre>

- This is the high pressure structure of BaZnF₄, stable above 5 GPa. (Posse, 2011).
- Data for this structure was taken at 6.81 GPa.
- (Posse, 2011) present the data in the Pn setting of space group #7. We use AFLOW to translate this into the standard Pc setting. This involves a reconfiguring of the lattice vectors.

Simple Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B}_2$	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Ba I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Ba II
$\mathbf{B}_4$	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Ba II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	F I
$\mathbf{B}_6$	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	F I
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	F II
$\mathbf{B}_8$	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	F II
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	F III
$\mathbf{B}_{10}$	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	F III
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	F IV
$\mathbf{B}_{12}$	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	F IV
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	F V
$\mathbf{B}_{14}$	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	F V
$\mathbf{B}_{15}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	F VI
$\mathbf{B}_{16}$	$x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	F VI
$\mathbf{B}_{17}$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	F VII

$$\begin{aligned}
\mathbf{B}_{18} &= x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_9 + c \left(z_9 + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + &(2a) & \text{F VII} \\
&&& c \left(z_9 + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{19} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= (ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}} &(2a) & \text{F VIII} \\
\mathbf{B}_{20} &= x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{10} + c \left(z_{10} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + &(2a) & \text{F VIII} \\
&&& c \left(z_{10} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{21} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= (ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}} &(2a) & \text{Zn I} \\
\mathbf{B}_{22} &= x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{11} + c \left(z_{11} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + &(2a) & \text{Zn I} \\
&&& c \left(z_{11} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= (ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}} &(2a) & \text{Zn II} \\
\mathbf{B}_{24} &= x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + \left(z_{12} + \frac{1}{2}\right) \mathbf{a}_3 &= \left(ax_{12} + c \left(z_{12} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + &(2a) & \text{Zn II} \\
&&& c \left(z_{12} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}
\end{aligned}$$

References

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