

BaZn₅ Structure:

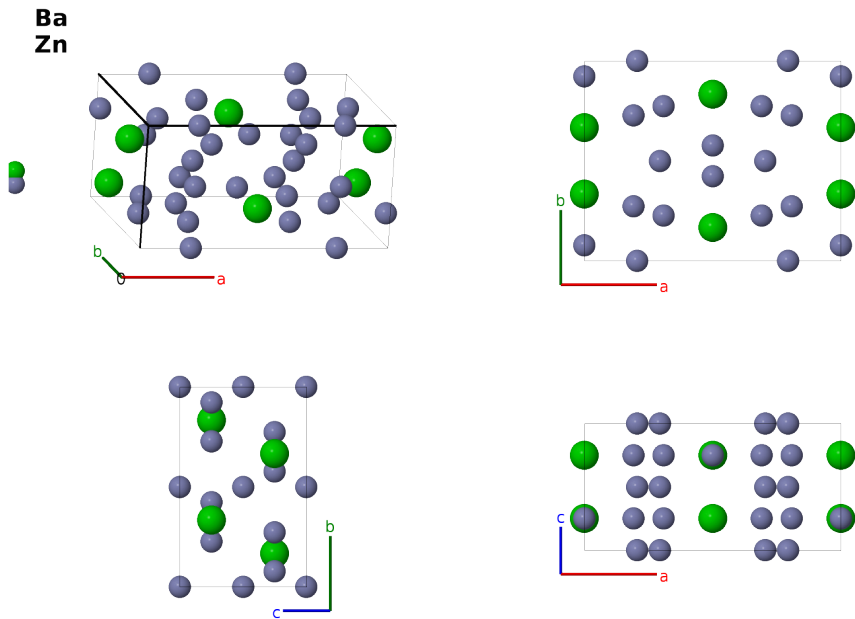
AB5_oC24_63_c_ceg-001

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<https://aflow.org/prototype-encyclopedia/BGG4>

https://aflow.org/prototype-encyclopedia/AB5_oC24_63_c_ceg-001



Prototype	BaZn ₅
AFLOW prototype label	AB5_oC24_63_c_ceg-001
ICSD	418610
CCDC	1731634
Pearson symbol	oC24
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=AB5_oC24_63_c_ceg-001</code> <code>--params=a, b/a, c/a, y₁, y₂, x₃, x₄, y₄</code>

Base-centered Orthorhombic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Ba I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Zn I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Zn I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}}$	(8e)	Zn II
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Zn II
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}}$	(8e)	Zn II
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8e)	Zn II
$\mathbf{B}_9$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{10}$	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{11}$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	Zn III
$\mathbf{B}_{12}$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	Zn III

References

- [1] M. Wendorff and C. Röhr, *Zink-reiche Erdalkalimetall-Verbindungen AZn_5 und AZn_{11} : Kristallstrukturen und chemische Bindung*, Z. Naturforsch. B **62**, 1549–1562 (2007), doi:10.1515/znb-2007-1213.

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