

SrZn₅ Structure:

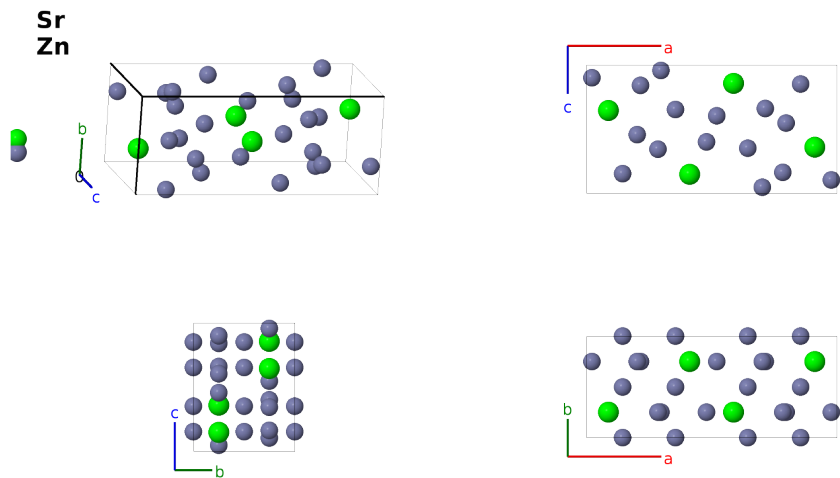
AB5_oP24_62_c_3cd-001

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<https://aflow.org/prototype-encyclopedia/BRA8>

https://aflow.org/prototype-encyclopedia/AB5_oP24_62_c_3cd-001

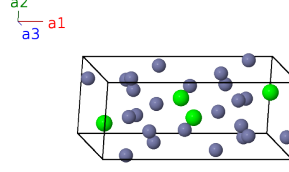


Prototype	SrZn ₅
AFLOW prototype label	AB5_oP24_62_c_3cd-001
ICSD	106115
CCDC	1663969
Pearson symbol	oP24
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<pre>aflow --proto=AB5_oP24_62_c_3cd-001 --params=a, b/a, c/a, x₁, z₁, x₂, z₂, x₃, z₃, x₄, z₄, x₅, y₅, z₅</pre>

- (Baenziger, 1956) give this structure in the *Pmcn* setting of space group #62. We used FINDSYM to place it in the standard *Pnma* setting.
- At high temperatures SrZn₅ transforms into the CaCu₅ (*D*_{2d}) structure. (Wendorff, 2007)
- This is the binary form of the SrAu₃Al₂ structure.

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Sr I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Sr I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Sr I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Sr I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Zn I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Zn I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Zn I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Zn I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Zn II
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Zn II
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	Zn II
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Zn II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Zn III
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Zn III
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	Zn III
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4c)	Zn III
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	Zn IV
$\mathbf{B}_{18}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	Zn IV
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8d)	Zn IV
$\mathbf{B}_{20}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	Zn IV
$\mathbf{B}_{21}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8d)	Zn IV
$\mathbf{B}_{22}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + y_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	Zn IV
$\mathbf{B}_{23}$	$= x_5 \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8d)	Zn IV
$\mathbf{B}_{24}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8d)	Zn IV

References

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- [2] 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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