

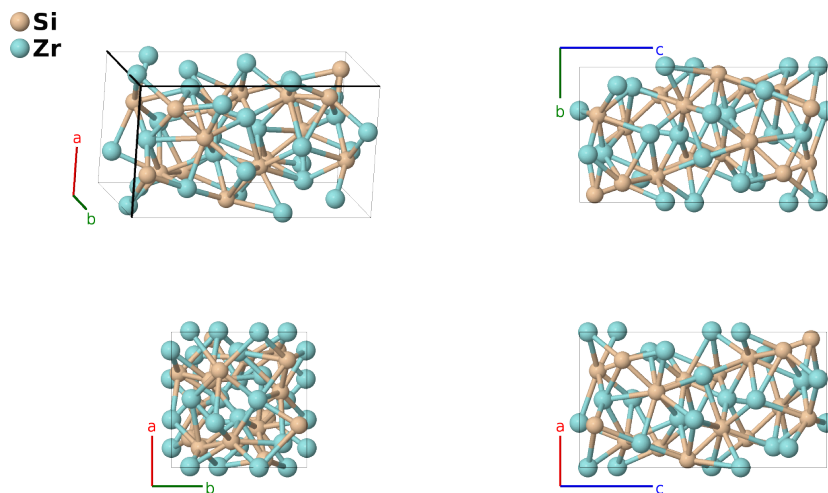
# Zr<sub>5</sub>Si<sub>4</sub> Structure:

## A4B5\_tP36\_92\_2b\_a2b-001

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<https://aflow.org/p/C3GS>

[https://aflow.org/p/A4B5\\_tP36\\_92\\_2b\\_a2b-001](https://aflow.org/p/A4B5_tP36_92_2b_a2b-001)



Prototype	Si <sub>4</sub> Zr <sub>5</sub>
AFLOW prototype label	A4B5_tP36_92_2b_a2b-001
ICSD	43214
Pearson symbol	tP36
Space group number	92
Space group symbol	$P4_12_12$
AFLOW prototype command	<code>aflow --proto=A4B5_tP36_92_2b_a2b-001</code> <code>--params=a, c/a, x<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub></code>

### Other compounds with this structure

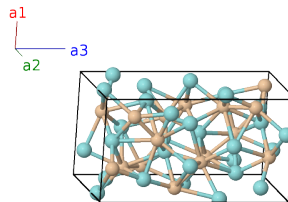
Ce<sub>5</sub>Si<sub>4</sub>, Hf<sub>5</sub>Si<sub>4</sub>, La<sub>5</sub>Si<sub>4</sub>, Nb<sub>5</sub>Si<sub>4</sub>, Pr<sub>5</sub>Si<sub>4</sub>, Ti<sub>5</sub>Si<sub>4</sub>, Zr<sub>5</sub>Ge<sub>4</sub>, Pr<sub>5</sub>Si<sub>2</sub>Ge<sub>2</sub>

### Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{x}$$

$$\mathbf{a}_2 = a \hat{y}$$

$$\mathbf{a}_3 = c \hat{z}$$



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}}$	(4a)	Zr I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B}_3$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4a)	Zr I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8b)	Si I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Si I
$\mathbf{B}_7$	$= -\left(y_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Si I
$\mathbf{B}_8$	$= \left(y_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_2 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Si I
$\mathbf{B}_9$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Si I
$\mathbf{B}_{10}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Si I
$\mathbf{B}_{11}$	$= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8b)	Si I
$\mathbf{B}_{12}$	$= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Si I
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B}_{14}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B}_{15}$	$= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B}_{16}$	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B}_{17}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B}_{18}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B}_{19}$	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B}_{20}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B}_{21}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8b)	Zr II
$\mathbf{B}_{22}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Zr II
$\mathbf{B}_{23}$	$= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Zr II
$\mathbf{B}_{24}$	$= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Zr II
$\mathbf{B}_{25}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	Zr II
$\mathbf{B}_{26}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	Zr II
$\mathbf{B}_{27}$	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8b)	Zr II
$\mathbf{B}_{28}$	$= -y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	Zr II
$\mathbf{B}_{29}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8b)	Zr III

$$\begin{aligned}
\mathbf{B}_{30} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8b) & \text{Zr III} \\
\mathbf{B}_{31} &= -\left(y_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 + &= -a \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Zr III} \\
&\quad \left(z_5 + \frac{1}{4}\right) \mathbf{a}_3 \\
\mathbf{B}_{32} &= \left(y_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 + &= a \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_5 + \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Zr III} \\
&\quad \left(z_5 + \frac{3}{4}\right) \mathbf{a}_3 \\
\mathbf{B}_{33} &= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - &= -a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Zr III} \\
&\quad \left(z_5 - \frac{1}{4}\right) \mathbf{a}_3 \\
\mathbf{B}_{34} &= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 - &= a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_5 - \frac{3}{4}\right) \hat{\mathbf{z}} & (8b) & \text{Zr III} \\
&\quad \left(z_5 - \frac{3}{4}\right) \mathbf{a}_3 \\
\mathbf{B}_{35} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= ay_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} & (8b) & \text{Zr III} \\
\mathbf{B}_{36} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= -ay_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8b) & \text{Zr III}
\end{aligned}$$

## References

- [1] H.-U. Pfeifer and K. Schubert, *Kristallstruktur von  $Zr_5S_4$* , Z. Metallkd. **57**, 884–888 (1966), doi:10.1515/ijmr-1966-571207.