

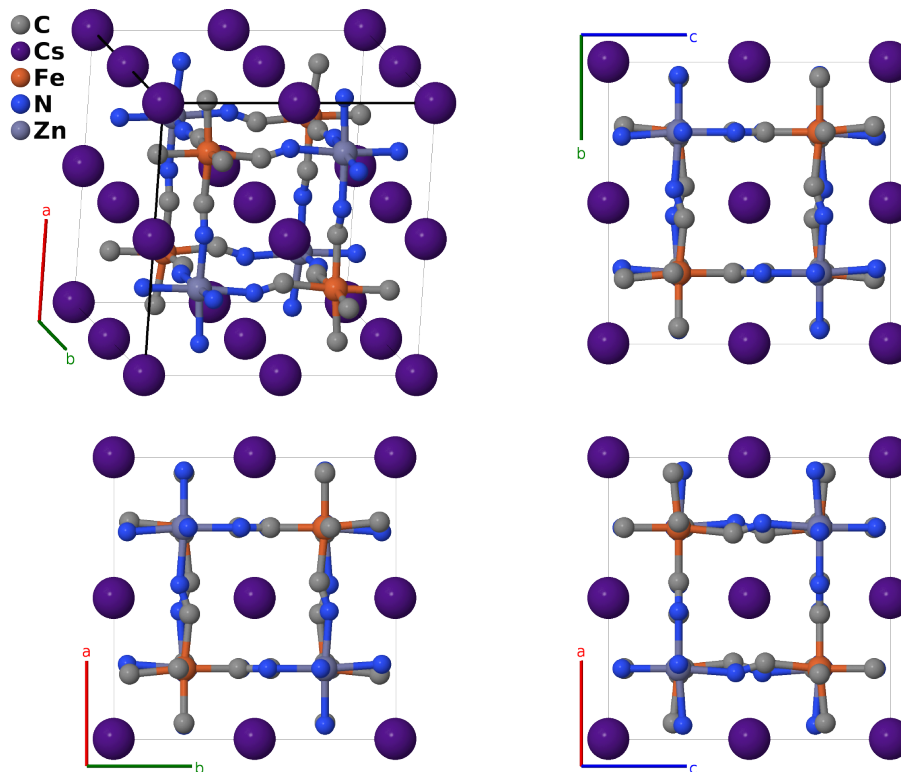
Cs₂ZnFe[CN]₆ Structure: A6B2CD6E_cP64_208_m_ad_b_m_c-001

This structure originally had the label A6B2CD6E_cP64_208_m_ad_b_m_c. Calls to that address will be redirected here.

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<https://aflow.org/p/0HGH>

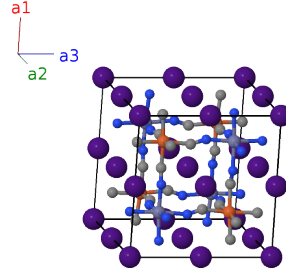
https://aflow.org/p/A6B2CD6E_cP64_208_m_ad_b_m_c-001



Prototype	C ₆ Cs ₂ FeN ₆ Zn
AFLOW prototype label	A6B2CD6E_cP64_208_m_ad_b_m_c-001
ICSD	None
Pearson symbol	cP64
Space group number	208
Space group symbol	<i>P</i> 4 ₂ 32
AFLOW prototype command	<code>aflow --proto=A6B2CD6E_cP64_208_m_ad_b_m_c-001 --params=a, x₅, y₅, z₅, x₆, y₆, z₆</code>

Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	Cs I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(2a)	Cs I
\mathbf{B}_3	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4b)	Fe I
\mathbf{B}_4	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4b)	Fe I
\mathbf{B}_5	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4b)	Fe I
\mathbf{B}_6	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4b)	Fe I
\mathbf{B}_7	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4c)	Zn I
\mathbf{B}_8	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(4c)	Zn I
\mathbf{B}_9	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4c)	Zn I
\mathbf{B}_{10}	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(4c)	Zn I
\mathbf{B}_{11}	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6d)	Cs II
\mathbf{B}_{12}	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6d)	Cs II
\mathbf{B}_{13}	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6d)	Cs II
\mathbf{B}_{14}	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(6d)	Cs II
\mathbf{B}_{15}	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(6d)	Cs II
\mathbf{B}_{16}	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(6d)	Cs II
\mathbf{B}_{17}	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{18}	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{19}	$-x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{20}	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{21}	$z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{22}	$z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{23}	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{24}	$-z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{25}	$y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{26}	$-y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{27}	$y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{28}	$-y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(24m)	C I
\mathbf{B}_{29}	$(y_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(24m)	C I

$$\begin{aligned}
\mathbf{B}_{58} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24m) & \text{N I} \\
\mathbf{B}_{59} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24m) & \text{N I} \\
\mathbf{B}_{60} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24m) & \text{N I} \\
\mathbf{B}_{61} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24m) & \text{N I} \\
\mathbf{B}_{62} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24m) & \text{N I} \\
\mathbf{B}_{63} &= -\left(z_6 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (24m) & \text{N I} \\
\mathbf{B}_{64} &= -\left(z_6 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_6 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (24m) & \text{N I}
\end{aligned}$$

References

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Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.
- [2] P. Villars, *$Cs_2ZnFe[CN]_6$ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.