

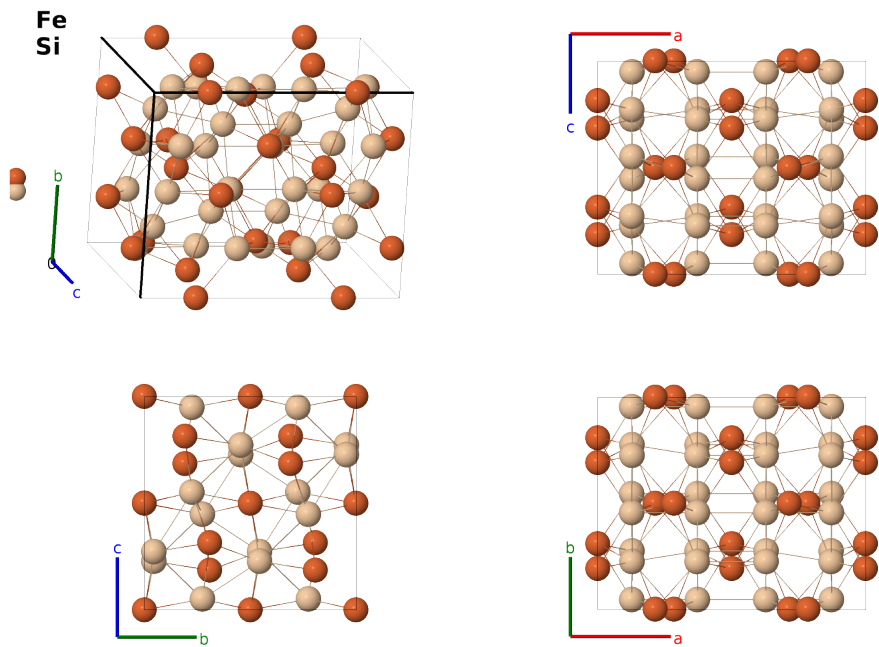
Low Temperature FeSi₂ Structure: AB2_oC48_64_df_2g-001

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<https://aflow.org/prototype-encyclopedia/MR28>

https://aflow.org/prototype-encyclopedia/AB2_oC48_64_df_2g-001



Prototype	FeSi ₂
AFLOW prototype label	AB2_oC48_64_df_2g-001
ICSD	9119
CCDC	1594170
Pearson symbol	oC48
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>aflow --proto=AB2_oC48_64_df_2g-001</code> <code>--params=a, b/a, c/a, x₁, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

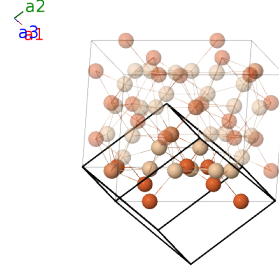
- This is the low temperature structure of FeSi₂. This transforms to the tetragonal high temperature structure above 962-1000K, with the exact temperature dependent up on the iron concentration in the high temperature phase. (Villars, 2018)

Base-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$$

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$a x_1 \hat{\mathbf{x}}$	(8d)	Fe I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-a x_1 \hat{\mathbf{x}}$	(8d)	Fe I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8d)	Fe I
$\mathbf{B}_5$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B}_6$	$= \left(y_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B}_7$	$= -\left(y_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B}_8$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-b y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8f)	Fe II
$\mathbf{B}_9$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B}_{10}$	$= \left(-x_3 + y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 + y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B}_{11}$	$= -\left(x_3 + y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(-x_3 + y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B}_{12}$	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B}_{13}$	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B}_{14}$	$= \left(x_3 - y_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B}_{15}$	$= \left(x_3 + y_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 - y_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B}_{16}$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16g)	Si I
$\mathbf{B}_{17}$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(16g)	Si II
$\mathbf{B}_{18}$	$= \left(-x_4 + y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 + y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16g)	Si II

$$\begin{aligned}
\mathbf{B}_{19} &= \begin{matrix} -(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_1 + \\ (-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (16g) & \text{Si II} \\
\mathbf{B}_{20} &= \begin{matrix} (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 - \\ z_4 \mathbf{a}_3 \end{matrix} = ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (16g) & \text{Si II} \\
\mathbf{B}_{21} &= \begin{matrix} -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - \\ z_4 \mathbf{a}_3 \end{matrix} = -ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (16g) & \text{Si II} \\
\mathbf{B}_{22} &= \begin{matrix} (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (16g) & \text{Si II} \\
\mathbf{B}_{23} &= \begin{matrix} (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}} & (16g) & \text{Si II} \\
\mathbf{B}_{24} &= \begin{matrix} -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \\ z_4 \mathbf{a}_3 \end{matrix} = -ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (16g) & \text{Si II}
\end{aligned}$$

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- [1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Iron-Silicon Binary Phase Diagram (1997 Lindholm M.). Copyright ©2006-2018 ASM International.

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