

# FeSi (*B*20) Structure: AB\_cP8\_198\_a\_a-002

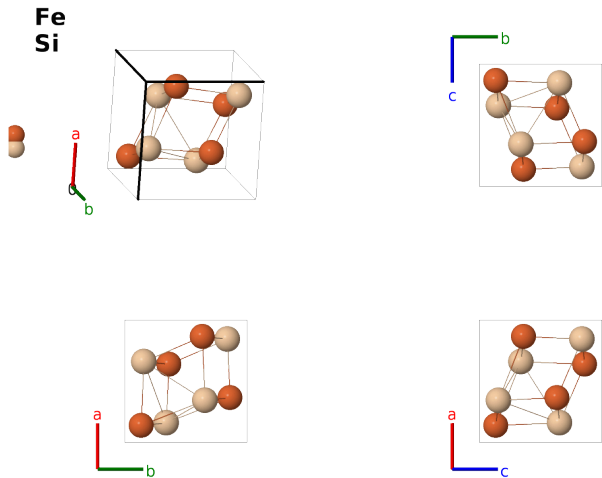
This structure previously used the label(s) **AB\_cP8\_198\_a\_a.FeSi**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/93P7>

[https://aflow.org/prototype-encyclopedia/AB\\_cP8\\_198\\_a\\_a-002](https://aflow.org/prototype-encyclopedia/AB_cP8_198_a_a-002)



|                                    |                                                                                                 |
|------------------------------------|-------------------------------------------------------------------------------------------------|
| Prototype                          | FeSi                                                                                            |
| AFLOW prototype label              | AB_cP8_198_a_a-002                                                                              |
| <i>Strukturbericht</i> designation | <i>B</i> 20                                                                                     |
| ICSD                               | 5250                                                                                            |
| CCDC                               | 1593316                                                                                         |
| Pearson symbol                     | cP8                                                                                             |
| Space group number                 | 198                                                                                             |
| Space group symbol                 | $P2_13$                                                                                         |
| AFLOW prototype command            | <code>aflow --proto=AB_cP8_198_a_a-002</code><br><code>--params=<math>a, x_1, x_2</math></code> |

## Other compounds with this structure

AlPt, AuBe, CoGe, CoSi, CrGe, CrSi, FeGe, FeSi, GaPd, GaPt, GeMn, GeRh, GeRu, HfSb, HfSn, HgPd, MgPt, MnGe, MnSi, OsSi, ReSi, RhS, RhSi, RhSn, RuGe, RuSi, SbZr, SiTc

- When  $x_1 = 0$  and  $x_2 = 1/2$ , or  $x_1 = 1/4$  and  $x_2 = 3/4$ , this lattice reduces to the rock salt (*B*1) structure. When  $x_1 = -x_2 = 1/8(\sqrt{5} - 1)$  we have an “idea” structure where every atom is seven-fold coordinated.

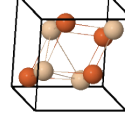
- FeSi (*B20*) and  $\alpha$ -CO (*B21*) have the same AFLOW prototype label, AB\_cP8\_198\_a\_a. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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### Simple Cubic primitive vectors

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

$\mathbf{a}_1$   
 $\mathbf{a}_2$   
 $\mathbf{a}_3$




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### Basis vectors

|                | Lattice<br>coordinates                                                                                            |     | Cartesian<br>coordinates                                                                                                       | Wyckoff<br>position | Atom<br>type |
|----------------|-------------------------------------------------------------------------------------------------------------------|-----|--------------------------------------------------------------------------------------------------------------------------------|---------------------|--------------|
| $\mathbf{B}_1$ | $= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$                                                        | $=$ | $ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$                                                        | (4a)                | Fe I         |
| $\mathbf{B}_2$ | $= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4a)                | Fe I         |
| $\mathbf{B}_3$ | $= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-ax_1 \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4a)                | Fe I         |
| $\mathbf{B}_4$ | $= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$  | $=$ | $a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$  | (4a)                | Fe I         |
| $\mathbf{B}_5$ | $= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$                                                        | $=$ | $ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$                                                        | (4a)                | Si I         |
| $\mathbf{B}_6$ | $= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4a)                | Si I         |
| $\mathbf{B}_7$ | $= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (4a)                | Si I         |
| $\mathbf{B}_8$ | $= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$  | $=$ | $a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$  | (4a)                | Si I         |

### References

- [1] L. Vočadlo, K. S. Knight, G. D. Price, and I. G. Wood, *Thermal expansion and crystal structure of FeSi between 4 and 1173 K determined by time-of-flight neutron powder diffraction*, Phys. Chem. Miner. **29**, 132–139 (2002), doi:10.1007/s002690100202.

### First cited in

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