# Linzhiite (High Temperature $FeSi_2$) Structure: AB2_tP3_123_a_h-001

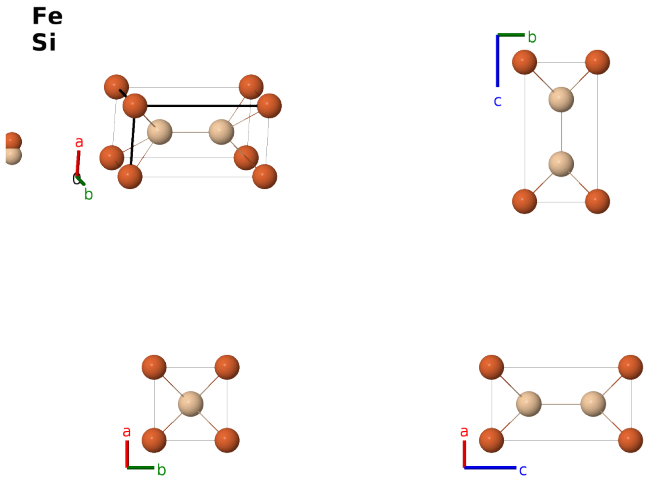
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/N538

https://aflow.org/prototype-encyclopedia/AB2_tP3_123_a_h-001



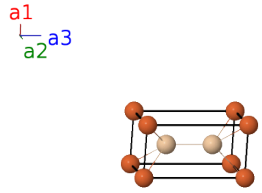

| | |
|---|---|
| **Prototype** | $FeSi_2$ |
| **AFLOW prototype label** | AB2_tP3_123_a_h-001 |
| **Mineral name** | linzhiite |
| **ICSD** | 24360 |
| **CCDC** | 1600400 |
| **Pearson symbol** | tP3 |
| **Space group number** | 123 |
| **Space group symbol** | $P4/mmm$ |
| **AFLOW prototype command** | `aflow --proto=AB2_tP3_123_a_h-001 --params=`$a, c/a, z_2$ |

---

- This is the high temperature structure of $FeSi_2$. The actual composition is $Fe_xSi_2$ with $x < 1$, and the transition temperature varies with composition between 962 and 1000K. (Villars, 2018) The low temperature structure is body-centered orthorhombic.

### Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




### Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (1a) | Fe I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (2h) | Si I |
| $\mathbf{B_3}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (2h) | Si I |

### References


[1] B. Aronson, *A Note on the Compositions and Crystal Structures of $MnB_2$, $Mn_3Si$, $Mn_5Si_3$, and $FeSi_2$*, Acta Chem. Scand. **14**, 1414–1418 (1960), doi:10.3891/acta.chem.scand.14-1414.


### Found in


[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.


### First cited in


H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.