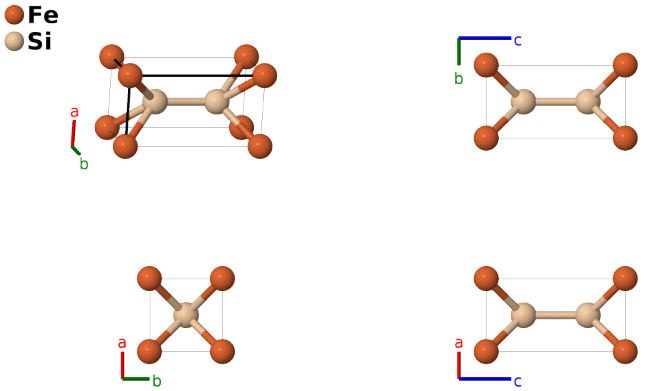
Linzhiite (High Temperature $FeSi_2$) Structure: AB2_tP3_123_a_h-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/N538

https://aflow.org/p/AB2_tP3_123_a_h-001

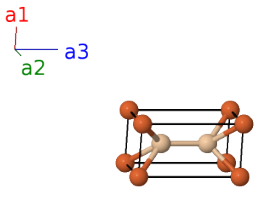


Prototype	$FeSi_2$
AFLOW prototype label	AB2_tP3_123_a_h-001
Mineral name	linzhiite
ICSD	24360
Pearson symbol	tP3
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=AB2_tP3_123_a_h-001 --params=`$a, c/a, z_2$

- 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.