

CsFeF₄ II Structure:

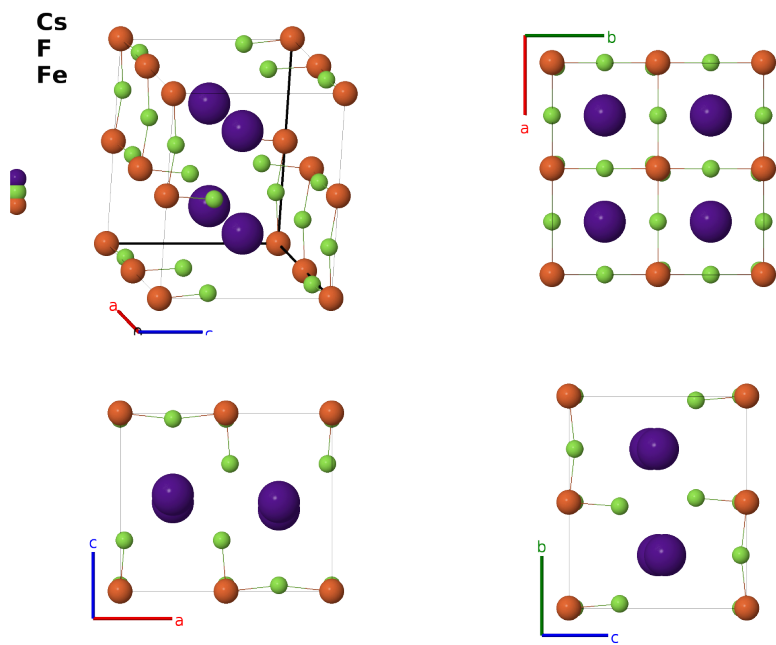
AB4C_tP24_129_bc_ij_d-001

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- 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/K69U>

https://aflow.org/prototype-encyclopedia/AB4C_tP24_129_bc_ij_d-001



Prototype	CsF ₄ Fe
AFLOW prototype label	AB4C_tP24_129_bc_ij_d-001
ICSD	62696
CCDC	1625906
Pearson symbol	tP24
Space group number	129
Space group symbol	<i>P4/nmm</i>
AFLOW prototype command	<code>aflow --proto=AB4C_tP24_129_bc_ij_d-001 --params=a, c/a, z₂, y₄, z₄, x₅, z₅</code>

Other compounds with this structure

CsMnF₄, CsTiF₄, CsVF₄

- (Hidaka, 1986) identify two phase transitions in CsFeF₄:

- At high temperatures, CsFeF_4 I has the tetragonal TlAlF_4 ($H0_8$) structure.
- At 475K there is a second-order phase transition to CsFeF_4 II, tetragonal space group $P4/nmm$ #129 (this structure).
- At 250K there is a second-order phase transition to CsFeF_4 III, orthorhombic space group $P2_12_12$ #18, with the RbAlF_4 III structure.

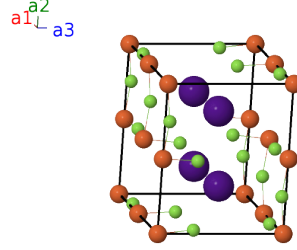
- The different structures are distinguished by the tilt of the FeF_6 octahedra.

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
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2b)	Cs I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2b)	Cs I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	Cs II
$\mathbf{B}_4$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2c)	Cs II
$\mathbf{B}_5$	$= 0$	$=$	0	(4d)	Fe I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$	(4d)	Fe I
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(4d)	Fe I
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{y}}$	(4d)	Fe I
$\mathbf{B}_9$	$= \frac{1}{4} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8i)	F I
$\mathbf{B}_{10}$	$= \frac{1}{4} \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8i)	F I
$\mathbf{B}_{11}$	$= -(y_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8i)	F I
$\mathbf{B}_{12}$	$= y_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ay_4 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8i)	F I
$\mathbf{B}_{13}$	$= \frac{3}{4} \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8i)	F I
$\mathbf{B}_{14}$	$= \frac{3}{4} \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8i)	F I
$\mathbf{B}_{15}$	$= (y_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8i)	F I
$\mathbf{B}_{16}$	$= -y_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ay_4 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8i)	F I
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8j)	F II
$\mathbf{B}_{18}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8j)	F II
$\mathbf{B}_{19}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8j)	F II
$\mathbf{B}_{20}$	$= x_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8j)	F II
$\mathbf{B}_{21}$	$= -x_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8j)	F II
$\mathbf{B}_{22}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(8j)	F II

$$\mathbf{B}_{23} = \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3 = a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} \quad (8j) \quad \text{F II}$$

$$\mathbf{B}_{24} = -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 = -ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} \quad (8j) \quad \text{F II}$$

References

- [1] M. Hidaka, H. Fujii, B. J. Garrard, and B. M. Wanklyn, *Structural phase transitions in the layer compound CsFeF₄*, Phys. Stat. Solidi A **95**, 413–421 (1986), doi:10.1002/pssa.2210950207.

Found in

- [1] M. Hidaka, H. Fujii, B. J. Garrard, and B. M. Wanklyn, *Structural Phase Transitions in the Layer Compound CsVF₄*, Phys. Stat. Solidi A **96**, 415–423 (1986), doi:10.1002/pssa.2210960206.

First cited in

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