FeF_3 ($D0_{12}$) Structure: A3B_hR8_167_e_b-001

This structure originally had the label `A3B_hR8_167_e_b`. Calls to that address will be redirected here.

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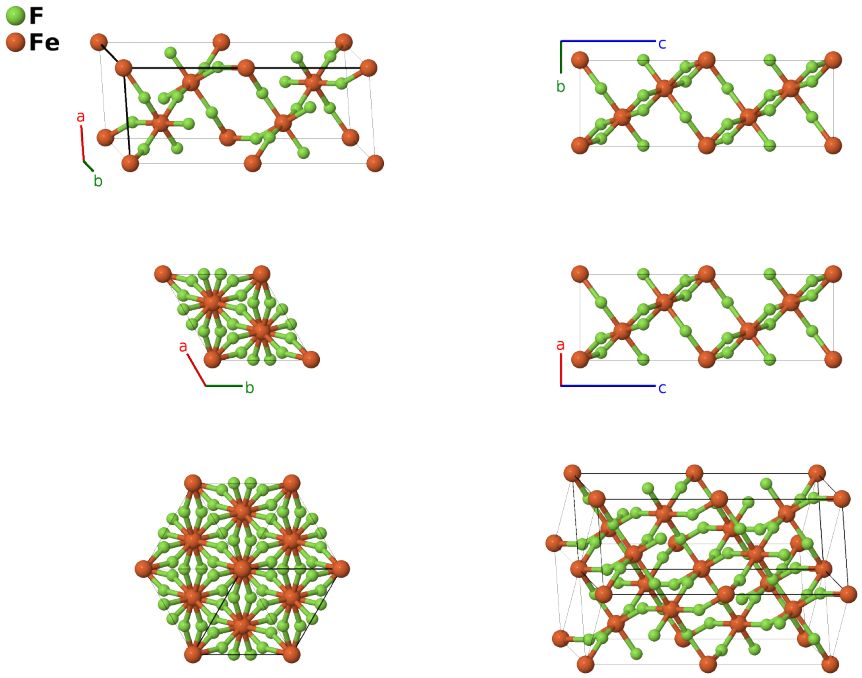
https://aflow.org/p/GPY3

https://aflow.org/p/A3B_hR8_167_e_b-001



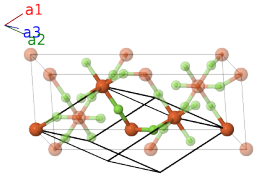
Prototype	F_3Fe
AFLOW prototype label	A3B_hR8_167_e_b-001
***Strukturbericht* designation**	$D0_{12}$
ICSD	16671
Pearson symbol	hR8
Space group number	167
Space group symbol	$R\bar{3}c$
AFLOW prototype command	`aflow --proto=A3B_hR8_167_e_b-001 --params=`$a, c/a, x_2$

Other compounds with this structure

α-AlF_3, AlH_3, CNi_3, CoF_3, CrF_3, GaF_3, IrF_3, MoF_3, PdF_3, RhF_3, RuF_3, ScF_3, TeO_3, VF_3, ZrO_3

Rhombohedral primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2b)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Fe I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_2-1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{8}a\,(4x_2-1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	F I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,(4x_2-1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{8}a\,(4x_2-1)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	F I
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6e)	F I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_2+3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{24}a\,(12x_2+1)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	F I
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{8}a\,(4x_2-1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{24}a\,(12x_2+5)\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	F I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{5}{12}c\,\hat{\mathbf{z}}$	(6e)	F I

References

[1] M. A. Hepworth, K. H. Jack, R. D. Peacock, and G. J. Westland, *The crystal structures of the trifluorides of iron, cobalt, ruthenium, rhodium, palladium and iridium*, Acta Cryst. **10**, 63–69 (1957), doi:10.1107/S0365110X57000158.