

FeF <sub>3</sub>	<i>hP</i> 24	(176) <i>P</i> 6 <sub>3</sub> / <i>m</i> – <i>ihg</i>
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**FeF<sub>3</sub> HTB It** [1]

Structural features: FeF<sub>6</sub> octahedra share vertices to form an HTB-type framework with channels parallel to [001]. Slightly distorted derivative of hexagonal WO<sub>3</sub>.

Leblanc M. et al. (1986) [1]

F<sub>3</sub>Fe

$a = 0.7402$ ,  $c = 0.7569$  nm,  $c/a = 1.023$ ,  $V = 0.3591$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	12 <i>i</i>	1	0.2111	0.4222	0.0		non-colinear Fe <sub>2</sub>
F2	6 <i>h</i>	<i>m</i> ..	0.029	0.496	<sup>1</sup> / <sub>4</sub>		non-colinear Fe <sub>2</sub>
Fe3	6 <i>g</i>	-1	<sup>1</sup> / <sub>2</sub>	0	0		octahedron F <sub>6</sub>

Transformation from published data: *y,x,-z*; origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.048, T = 4.2 K

Remarks: Phase stable at T < ~97 K.

References: [1] Leblanc M., De Pape R., Ferey G., Pannetier J. (1986), Solid State Commun. 58, 171-176.