

$(\text{Mn}_{0.33}\text{Fe}_{0.67})_3\text{Pb}_2\text{F}_{12}[\text{H}_2\text{O}]_3$ *hP20*(189) *P*-62*m* – $\text{jg}^2\text{f}^2\text{d}$ **Pb₂MnFe₂F₁₂·3H₂O** [1]

Structural features: Triple infinite chains of vertex-linked (Fe,Mn)F₆ octahedra share vertices with PbF₆ trigonal prisms to form a 3D-framework; H₂O in channels of pentagonal cross-section parallel to [001].

Le Bail A., Mercier A.M. (1992) [1]

 $\text{F}_{12}\text{Fe}_2\text{H}_6\text{MnO}_3\text{Pb}_2$ $a = 0.932$, $c = 0.39618$ nm, $c/a = 0.425$, $V = 0.2980$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	6 <i>j</i>	<i>m</i> ..	0.1797	0.4707	0		single atom Fe
F2	3 <i>g</i>	<i>m2m</i>	0.2391	0	$\frac{1}{2}$		non-colinear Fe ₂
(OH ₂)3	3 <i>g</i>	<i>m2m</i>	0.5919	0	$\frac{1}{2}$		15-vertex polyhedron Pb ₂ F ₁₃
M4	3 <i>f</i>	<i>m2m</i>	0.2401	0	0		octahedron F ₆
F5	3 <i>f</i>	<i>m2m</i>	0.823	0	0		non-colinear Fe ₂
Pb6	2 <i>d</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism F ₆ (OH ₂) ₃

 $\text{M4} = 0.667\text{Fe} + 0.333\text{Mn}$ Transformation from published data: -*x*, -*y*, -*z*Experimental: single crystal, diffractometer, X-rays, $R = 0.032$

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Le Bail A., Mercier A.M. (1992), Acta Crystallogr. C 48, 239-241.