

Fe₂[PHO₃]₃*hP*28(176) *P*6₃/*m* – ih²f**Fe₂(HPO₃)₃** [1]

Structural features: Units of two face-linked FeO₆ octahedra share vertices with P(HO₃) tetrahedra to form a 3D-framework.

Sghyar M. et al. (1991) [1]

Fe₂H₃O₉P₃*a* = 0.8037, *c* = 0.7352 nm, *c/a* = 0.915, *V* = 0.4113 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.4324	0.163	0.0784		non-colinear PFe
O2	6 <i>h</i>	<i>m</i> ..	0.1295	0.5124	¹ / ₄		single atom P
P3	6 <i>h</i>	<i>m</i> ..	0.3542	0.0464	¹ / ₄		non-coplanar triangle O ₃
Fe4	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.04826		octahedron O ₆
H5	6 <i>h</i>	<i>m</i> ..	0.0266	0.1826	¹ / ₄		

Transformation from published data: origin shift 0 0 ¹/₂Experimental: single crystal, diffractometer, X-rays, *R* = 0.028

Remarks: In [1] the number of formula units per cell *Z* is misprinted as 4 instead of 2. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Sghyar M., Durand J., Cot L., Rafiq M. (1991), Acta Crystallogr. C 47, 2515-2517.