

FeB[PO₄]₂[H₂O]₃*hP*90(178) *P*6₁22 – *c*⁶*b*³**Fe(H₂O)₂[BP₂O₈]·H₂O** [1]

Structural features: BO₄ and PO₄ tetrahedra share vertices to form infinite twisted chains, which are interconnected via Fe(O₄[OH₂]₂) octahedra to form a 3D-framework; additional H₂O in channels of hexagonal cross-section parallel to [001].

Yilmaz A. et al. (2000) [1]

BFeH₆O₁₁P₂*a* = 0.94583, *c* = 1.5707 nm, *c/a* = 1.661, *V* = 1.2169 nm³, *Z* = 6

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>c</i>	1	0.0668	0.386	0.0479		single atom P
O2	12 <i>c</i>	1	0.1886	0.2116	0.06423		non-colinear BP
P3	12 <i>c</i>	1	0.2157	0.3844	0.08093		tetrahedron O ₄
O4	12 <i>c</i>	1	0.3745	0.513	0.04153		single atom P
O5	12 <i>c</i>	1	0.4138	0.1784	0.01217		non-colinear BP
(OH ₂)6	12 <i>c</i>	1	0.4843	0.1951	0.4495		single atom Fe
B7	6 <i>b</i>	..2	0.1508	0.3017	¹ / ₄		tetrahedron O ₄
Fe8	6 <i>b</i>	..2	0.4471	0.8942	¹ / ₄		octahedron O ₄ (OH ₂) ₂
(OH ₂)9	6 <i>b</i>	..2	0.911	0.822	¹ / ₄		non-colinear (OH ₂) ₂

Transformation from published data (*P*6₅22): new axes -*a*,-*b*,-*c*; origin shift 0 0 ¹/₂Experimental: single crystal, diffractometer, X-rays, *R* = 0.030

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

References: [1] Yilmaz A., Bu X., Kizilyalli M., Stucky G.D. (2000), Chem. Mater. 12, 3243-3245.