

Al[PO₄][H₂O]_{2.34}*hP*186(185) *P6₃cm* – d¹¹c⁹**AlPO₄·xH₂O VPI-5 ht** [1], zeolite VFI hydrated htStructural features: AlO₄ and PO₄ tetrahedra share vertices to form a VFI-type zeolite framework; disordered arrangement of H₂O in channels delimited by 18-rings parallel to [001].

De Onate Martinez J. et al. (1998) [1]

AlH_{4.68}O_{6.34}P*a* = 1.89468, *c* = 0.81524 nm, *c/a* = 0.430, *V* = 2.5345 nm³, *Z* = 18

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH ₂)1	12 <i>d</i>	1	0.083	0.2934	0.4767	0.39	non-colinear (OH ₂) ₂
(OH ₂)2	12 <i>d</i>	1	0.0874	0.1789	0.0847	0.45	non-colinear (OH ₂) ₂
O3	12 <i>d</i>	1	0.1108	0.4341	0.0804		non-colinear PAI
O4	12 <i>d</i>	1	0.1678	0.5015	0.3447		non-colinear PAI
(OH ₂)5	12 <i>d</i>	1	0.1702	0.3268	0.3947	0.57	non-colinear (OH ₂) ₂
P6	12 <i>d</i>	1	0.1858	0.5025	0.1639		tetrahedron O ₄
O7	12 <i>d</i>	1	0.2056	0.5835	0.0866		non-colinear PAI
O8	12 <i>d</i>	1	0.2581	0.4897	0.1481		non-colinear PAI
(OH ₂)9	12 <i>d</i>	1	0.2646	0.379	0.2457	0.51	non-coplanar triangle (OH ₂)O ₂
Al10	12 <i>d</i>	1	0.3493	0.5202	0.051		tetrahedron O ₄
O11	12 <i>d</i>	1	0.382	0.4564	0.1232		non-colinear PAI
(OH ₂)12	6 <i>c</i>	.. <i>m</i>	0.0767	0	0.0187	0.49	non-colinear (OH ₂) ₂
(OH ₂)13	6 <i>c</i>	.. <i>m</i>	0.129	0	0.4457	0.32	non-coplanar triangle (OH ₂) ₃
(OH ₂)14	6 <i>c</i>	.. <i>m</i>	0.219	0	0.4047	0.37	non-coplanar triangle (OH ₂) ₃
(OH ₂)15	6 <i>c</i>	.. <i>m</i>	0.2909	0	0.0		single atom Al
(OH ₂)16	6 <i>c</i>	.. <i>m</i>	0.3376	0	0.3109		single atom Al
Al17	6 <i>c</i>	.. <i>m</i>	0.3837	0	0.0841		octahedron O ₄ (OH ₂) ₂
O18	6 <i>c</i>	.. <i>m</i>	0.4687	0	0.187		non-colinear PAI
P19	6 <i>c</i>	.. <i>m</i>	0.5494	0	0.2061		tetrahedron O ₄
O20	6 <i>c</i>	.. <i>m</i>	0.572	0	0.3869		non-colinear PAI

Transformation from published data: origin shift 0 0 0.1553

Experimental: powder, diffractometer, X-rays, synchrotron, wR_p = 0.098, T = 363 K

Remarks: Phase stable at T > 353 K. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] De Onate Martinez J., McCusker L.B., Baerlocher C., Engelhardt G. (1998), Microporous Mesoporous Mater. 22, 127-134.