$Al[PO_4][H_2O]_{2.53}$	*hP*204	(185) $P6_3cm$ – $d^{13}c^8$

$Al_{1.07}PO_4 \cdot 0.75H_2O \cdot 0.12$(TBA,DPTA) [1], zeolite VFI hydrated
Structural features: AlO_4 and PO_4 tetrahedra share vertices to form a VFI-type zeolite framework and a related framework with rotated 6-rings (partial disorder); H_2O in channels delimited by 18-rings parallel to [001].

Poojary D.M., Clearfield A. (1993) [1]
$AlH_{5.07}O_{6.53}P$
a = 1.89702, c = 0.81163 nm, c/a = 0.428, V = 2.5295 nm^3, Z = 18

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	12*d*	1	0.1048	0.4218	0.181	0.25	
O2	12*d*	1	0.1105	0.4301	0.107	0.75	
(OH_2)3	12*d*	1	0.116	0.296	0.429		single atom (OH_2)
O4	12*d*	1	0.1833	0.5008	0.371	0.75	non-coplanar triangle POAl
P5	12*d*	1	0.1853	0.5023	0.189		
(OH_2)6	12*d*	1	0.1923	0.3139	0.278		single atom (OH_2)
O7	12*d*	1	0.1956	0.5741	0.267	0.25	non-coplanar triangle O_2P
O8	12*d*	1	0.2037	0.5813	0.099	0.75	non-coplanar square O_2PAl
O9	12*d*	1	0.2575	0.488	0.141		non-coplanar triangle PAl_2
O10	12*d*	1	0.3373	0.5234	0.463	0.25	single atom O
Al11	12*d*	1	0.3412	0.5153	0.26	0.25	trigonal bipyramid O_4Al
Al12	12*d*	1	0.3525	0.5217	0.056	0.75	trigonal bipyramid O_4Al
O13	12*d*	1	0.3849	0.4598	0.134		non-coplanar triangle PAl_2
(OH_2)14	6*c*	..*m*	0.084	0	0.065	0.6	non-coplanar square $(OH_2)_4$
(OH_2)15	6*c*	..*m*	0.142	0	0.446		non-coplanar square $(OH_2)_4$
(OH_2)16	6*c*	..*m*	0.2928	0	0.0		single atom Al
(OH_2)17	6*c*	..*m*	0.3519	0	0.329		single atom Al
Al18	6*c*	..*m*	0.3857	0	0.108		
O19	6*c*	..*m*	0.4671	0	0.226		non-colinear PAl
P20	6*c*	..*m*	0.5511	0	0.232		tetrahedron O_4
O21	6*c*	..*m*	0.572	0	0.409		non-colinear PAl

Transformation from published data: origin shift 0 0 0.129
Experimental: powder, diffractometer, X-rays, synchrotron, R_p = 0.088

Remarks: Guest molecules not located. Short interatomic distances: d((OH_2)3-(OH_2)6) = 0.180 nm. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (173) $P6_3$ was tested and rejected.

References: [1] Poojary D.M., Clearfield A. (1993), Zeolites 13, 542-548.