

Al[PO ₄]	<i>hP</i> 168	(184) <i>P6cc</i> – d ¹⁴
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AlPO₄ form 5 [1], zeolite AFI

Structural features: AlO₄ and PO₄ tetrahedra share vertices to form an AFI-type zeolite framework with channels delimited by 12-rings parallel to [001] (3-fold disorder).

Klap G.J. et al. (2000) [1]

AlO₄P

$a = 1.3718$, $c = 0.84526$ nm, $c/a = 0.616$, $V = 1.3775$ nm³, $Z = 12$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.001	0.368	0.1077	0.333	
O2	12 <i>d</i>	1	0.005	0.353	0.0817	0.333	
O3	12 <i>d</i>	1	0.016	0.38	0.0357	0.333	
O4	12 <i>d</i>	1	0.091	0.436	0.2997	0.333	
P5	12 <i>d</i>	1	0.123	0.4526	0.12718		
O6	12 <i>d</i>	1	0.134	0.434	0.3007	0.333	
O7	12 <i>d</i>	1	0.14	0.49	0.2997	0.333	
O8	12 <i>d</i>	1	0.147	0.57	0.1017	0.333	
O9	12 <i>d</i>	1	0.152	0.558	0.0207	0.333	
O10	12 <i>d</i>	1	0.162	0.573	0.0757	0.333	
O11	12 <i>d</i>	1	0.202	0.409	0.0797	0.333	
O12	12 <i>d</i>	1	0.204	0.43	0.0337	0.333	
O13	12 <i>d</i>	1	0.421	0.208	0.1047	0.333	
Al14	12 <i>d</i>	1	0.4565	0.1206	0.0		

Transformation from published data: origin shift 0 0 0.9253

Experimental: single crystal, diffractometer, X-rays, wR = 0.043

Remarks: Disordered arrangement of three types of microdomain exhibiting symmetry (168) P6. Short interatomic distances for partly occupied site(s). The average structure without site splitting was also refined.

References: [1] Klap G.J., Van Koningsveld H., Graafsma H., Schreurs A.M.M. (2000), Microporous Mesoporous Mater. 38, 403-412.