

$\text{Al}_{12}[\text{SiO}_4][\text{PO}_4]_{11}\text{F}$	<i>hP78</i>	(184) <i>P6cc</i> – $d^6c$
--	-------------	----------------------------

**$\text{AlPO}_4\text{:SiO}_2$ , HF form 5** [1], zeolite AFI

Structural features:  $\text{AlO}_4$  and  $(\text{P,Si})\text{O}_4$  tetrahedra share vertices to form an AFI-type zeolite framework with channels delimited by 12-rings parallel to [001]; F above 4-rings.

Zhao D.Q. et al. (1992) [1]

$\text{Al}_{12}\text{FO}_{48}\text{P}_{11}\text{Si}$

$a = 1.3802$ ,  $c = 0.8503$  nm,  $c/a = 0.616$ ,  $V = 1.4028$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.0039	0.3626	0.1832		non-colinear PAI
O2	12 <i>d</i>	1	0.1245	0.454	0.421		non-colinear PAI
M3	12 <i>d</i>	1	0.1255	0.4532	0.2351		tetrahedron O <sub>4</sub>
O4	12 <i>d</i>	1	0.1557	0.566	0.1762		non-colinear PAI
O5	12 <i>d</i>	1	0.2055	0.4196	0.1898		non-colinear PAI
Al6	12 <i>d</i>	1	0.4556	0.1185	0.1071		tetrahedron O <sub>4</sub>
F7	6 <i>c</i>	2..	$\frac{1}{2}$	0	0.0	0.167	coplanar square Al <sub>2</sub> O <sub>2</sub>

$\text{M3} = 0.917\text{P} + 0.083\text{Si}$

Transformation from published data: origin shift 0 0 0.8179

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

Remarks: The authors state that Si substitutes exclusively for P. We assigned an approximate value to the P/Si ratio of site M3 based on the nominal composition.

References: [1] Zhao D.Q., Pang W.Q., Li L., Yang G.D. (1992), Gaodeng Xuexiao Huaxue Xuebao 13, 1165-1167.