

Al[PO <sub>4</sub> ]	<i>hP</i> 12	(186) <i>P</i> 6 <sub>3</sub> <i>mc</i> – cb <sup>3</sup>
----------------------	--------------	---

**AlPO<sub>4</sub> tridymite-type ht [1]**

Structural features: AlO<sub>4</sub> and PO<sub>4</sub> tetrahedra share vertices to form a 3D-framework with channels delimited by 6-rings parallel to [001]. Substitution derivative of SiO<sub>2</sub> tridymite.

Graetsch H.A. (2001) [1]

AlO<sub>4</sub>P

$a = 0.50976$ ,  $c = 0.83441$  nm,  $c/a = 1.637$ ,  $V = 0.1878$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>c</i>	. <i>m</i> .	0.5109	0.4891	0.4411		colinear PAI
P2	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0		tetrahedron O <sub>4</sub>
O3	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.1749		colinear PAI
Al4	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.374		tetrahedron O <sub>4</sub>

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.0635

Experimental: powder, diffractometer, X-rays, R<sub>p</sub> = 0.013, T = 593 K

Remarks: Phase stable at T > 573 K. Space group (159) *P*31*c* was tested and rejected; refinement of an alternative model considering multiple splitting of the O sites gave better interatomic distances.

References: [1] Graetsch H.A. (2001), Acta Crystallogr. C 57, 665-667.