

Al[PO₄]*hP*52(186) *P*6₃*mc* – d⁴b²**AlPO₄ tridymite-type ht** [1]

Structural features: AlO₄ and PO₄ tetrahedra share vertices to form a 3D-framework with channels delimited by 6-rings parallel to [001] (6-fold splitting of the O sites about the P-P axes). Substitution derivative of SiO₂ tridymite.

Graetsch H.A. (2001) [1]

AlO_{4.01}P*a* = 0.50976, *c* = 0.83441 nm, *c/a* = 1.637, *V* = 0.1878 nm³, *Z* = 2

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------------|-------------|-----------------------------|-----------------------------|----------|-------|--------------------|
| O1 | 12 <i>d</i> | 1 | 0.0028 | 0.4583 | 0.1063 | 0.167 | |
| O2 | 12 <i>d</i> | 1 | 0.4285 | 0.0252 | 0.0643 | 0.167 | |
| O3 | 12 <i>d</i> | 1 | 0.4837 | 0.052 | 0.0243 | 0.167 | |
| O4 | 12 <i>d</i> | 1 | 0.5859 | 0.2524 | 0.2994 | 0.167 | |
| Al5 | 2 <i>b</i> | 3 <i>m.</i> | ¹ / ₃ | ² / ₃ | 0.0 | | |
| P6 | 2 <i>b</i> | 3 <i>m.</i> | ¹ / ₃ | ² / ₃ | 0.6249 | | |

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.4375Experimental: powder, diffractometer, X-rays, *R*_p = 0.013, *T* = 593 K

Remarks: Phase stable at *T* > 573 K. Short interatomic distances for partly occupied site(s). Space group (159) *P*31*c* was tested and rejected. Refinement of an alternative model considering ideal O sites gave similar reliability factors but less realistic interatomic distances.

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