

Cs₉Mo₉Al₃[PO₄]₁₁O₁₅*hP*196(176) *P*6₃/*m* – i¹⁰h¹⁰f⁴**Cs₉Mo₉Al₃P₁₁O₅₉** [1]; Cs₇K₂Mo₉Al₃P₁₁O₅₉ [2]

Structural features: Units of three edge- and vertex-linked MoO₆ octahedra share vertices with Al₃P₁₀O₄₀ units (vertex-linked AlO₄ and PO₄ tetrahedra; orientational disorder up-down for the central PO₄ tetrahedron) and additional PO₄ tetrahedra to form a 3D-framework; Cs in large channels parallel to [001].

Guesdon A. et al. (1995) [1]

Al₃Cs₉Mo₉O₅₉P₁₁*a* = 1.6989, *c* = 1.1866 nm, *c/a* = 0.698, *V* = 2.9660 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cs1	12 <i>i</i>	1	0.14693	0.61941	0.04617		non-colinear O ₂
O2	12 <i>i</i>	1	0.1603	0.446	0.0811		single atom P
O3	12 <i>i</i>	1	0.1699	0.0205	0.1241		single atom Mo
Cs4	12 <i>i</i>	1	0.17076	0.19754	0.2356	0.5	
Mo5	12 <i>i</i>	1	0.27908	0.04499	0.1396		octahedron O ₆
O6	12 <i>i</i>	1	0.3025	0.2713	0.0014		single atom P
O7	12 <i>i</i>	1	0.3402	0.1478	0.0243		single atom P
P8	12 <i>i</i>	1	0.3778	0.2498	0.0183		tetrahedron O ₄
O9	12 <i>i</i>	1	0.413	0.0587	0.1446		single atom P
O10	12 <i>i</i>	1	0.4308	0.299	0.1223		non-colinear PAl
O11	6 <i>h</i>	<i>m</i> ..	0.058	0.3114	¹ / ₄		non-coplanar triangle Mo ₃
O12	6 <i>h</i>	<i>m</i> ..	0.0698	0.4822	¹ / ₄		single atom P
Mo13	6 <i>h</i>	<i>m</i> ..	0.1687	0.44017	¹ / ₄		octahedron O ₆
O14	6 <i>h</i>	<i>m</i> ..	0.2456	0.4063	¹ / ₄		single atom Mo
O15	6 <i>h</i>	<i>m</i> ..	0.2578	0.5747	¹ / ₄		
O16	6 <i>h</i>	<i>m</i> ..	0.3193	0.14	¹ / ₄		non-colinear Mo ₂
P17	6 <i>h</i>	<i>m</i> ..	0.4469	0.0331	¹ / ₄		tetrahedron O ₄
Al18	6 <i>h</i>	<i>m</i> ..	0.4873	0.3322	¹ / ₄		tetrahedron O ₄
O19	6 <i>h</i>	<i>m</i> ..	0.5509	0.0822	¹ / ₄		non-colinear PAl
O20	6 <i>h</i>	<i>m</i> ..	0.5722	0.3055	¹ / ₄		
O21	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.088	0.5	single atom P
P22	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.2138	0.5	
O23	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.579	0.5	single atom P
P24	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.7057	0.5	

Transformation from published data: *y*, *x*, -*z*

Experimental: single crystal, diffractometer, X-rays, wR = 0.033, T = 294 K

Remarks: A partly disordered arrangement of Cs and K is reported for Cs₇K₂Mo₉Al₃P₁₁O₅₉.

References: [1] Guesdon A., Borel M.M., Leclaire A., Grandin A., Raveau B. (1995), J. Solid State Chem. 114, 451-458. [2] Guesdon A., Leclaire A., Borel M.M., Raveau B. (1995), Chem. Mater. 7, 1873-1878.