

Rb₉Mo₉Al₃[PO₄]₁₁O₁₅

hP234

(176) $P6_3/m - i^{13}h^{10}f^4b$ **Rb₉Mo₉Al₃P₁₁O₅₉** [1]

Structural features: Units of three edge- and vertex-linked MoO₆ octahedra (partial disorder) 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; Rb in large channels parallel to [001].

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

Al₃Mo₉O₅₉P₁₁Rb₉ $a = 1.671$, $c = 1.19$ nm, $c/a = 0.712$, $V = 2.8776$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.033	0.309	0.0		single atom P
Rb2	12i	1	0.1425	0.18	0.146	0.25	
Rb3	12i	1	0.1507	0.619	0.0422	0.95	non-colinear O ₂
O4	12i	1	0.155	0.003	0.129	0.5	
O5	12i	1	0.1626	0.452	0.081		single atom P
Rb6	12i	1	0.1853	0.2153	0.2193	0.25	
O7	12i	1	0.194	0.041	0.125	0.5	
Mo8	12i	1	0.2732	0.0439	0.1434	0.5	
Mo9	12i	1	0.2969	0.0521	0.1379	0.5	
O10	12i	1	0.349	0.148	0.02		single atom P
P11	12i	1	0.3815	0.2509	0.0158		tetrahedron O ₄
O12	12i	1	0.4202	0.0613	0.143		single atom P
O13	12i	1	0.434	0.3	0.12		non-colinear PAl
O14	6h	m..	0.055	0.311	$\frac{1}{4}$		
O15	6h	m..	0.07	0.486	$\frac{1}{4}$		single atom P
Mo16	6h	m..	0.1694	0.4424	$\frac{1}{4}$		octahedron O ₆
O17	6h	m..	0.242	0.401	$\frac{1}{4}$		single atom Mo
O18	6h	m..	0.261	0.576	$\frac{1}{4}$		
O19	6h	m..	0.328	0.145	$\frac{1}{4}$		
P20	6h	m..	0.4522	0.0348	$\frac{1}{4}$		tetrahedron O ₄
Al21	6h	m..	0.4813	0.3262	$\frac{1}{4}$		tetrahedron O ₄
O22	6h	m..	0.557	0.086	$\frac{1}{4}$		non-colinear PAl
O23	6h	m..	0.572	0.302	$\frac{1}{4}$		non-coplanar triangle P ₂ Al
O24	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.089	0.5	single atom P
P25	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.218	0.5	
O26	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.573	0.5	single atom P
P27	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.692	0.5	trigonal bipyramid PO ₄
Rb28	2b	-3..	0	0	0	0.3	octahedron O ₆

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

Experimental: single crystal, diffractometer, X-rays, R = 0.062

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Guesdon A., Leclaire A., Borel M.M., Raveau B. (1995), Chem. Mater. 7, 1873-1878.