$H_6Rb_6(V_{0.5}Mo_{0.5})_6Mo_6[PO_4]_{13}O_6[OH]_9[H_2O]_{8.5}$	*hP*222	(176) $P6_3/m$ – $i^{11}h^{13}f^2ba$

$Rb_6[(Mo_9V_3O_6)(PO_4)_{10}(H_2PO_4)_3(OH)_9]\cdot 8.5H_2O$ [1]
Structural features: Units of four edge- and vertex-linked $Mo(O_4[OH]_2)$ and $(Mo,V)(O_5[OH])$ octahedra share vertices with PO_4 and $P(O_2[OH]_2)$ tetrahedra (in part orientational disorder up-down) to form a 3D-framework; Rb and H_2O in large channels parallel to [001].

Soghomonian V. et al. (1998) [1]
$H_{32}Mo_9O_{75.50}P_{13}Rb_6V_3$
a = 1.6563, c = 1.2534 nm, c/a = 0.757, V = 2.9778 nm^3, Z = 2

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
$(OH_2)1$	12*i*	1	0.0179	0.5354	0.0743	0.773	
O2	12*i*	1	0.0331	0.3056	0.0206		single atom P
Rb3	12*i*	1	0.1046	0.6143	0.0754		
P4	12*i*	1	0.1307	0.3836	0.0		tetrahedron O_4
O5	12*i*	1	0.1673	0.4498	0.0949		non-colinear PMo
(OH)6	12*i*	1	0.1722	0.2208	0.1574		single atom P
O7	12*i*	1	0.1822	0.043	0.1317		single atom Mo
Mo8	12*i*	1	0.2902	0.0561	0.1453		octahedron $O_4(OH)_2$
O9	12*i*	1	0.3475	0.1499	0.0215		single atom P
O10	12*i*	1	0.4292	0.0737	0.1478		non-colinear $P(OH_2)$
O11	12*i*	1	0.4413	0.308	0.0949		non-colinear PMo
(OH)12	6*h*	*m*..	0.0428	0.3086	$^1/_4$		non-coplanar triangle Mo_3
O13	6*h*	*m*..	0.0654	0.4866	$^1/_4$		non-colinear PMo
M14	6*h*	*m*..	0.1573	0.4428	$^1/_4$		octahedron $O_5(OH)$
P15	6*h*	*m*..	0.234	0.2928	$^1/_4$		tetrahedron $O_2(OH)_2$
O16	6*h*	*m*..	0.2366	0.3856	$^1/_4$		single atom P
O17	6*h*	*m*..	0.272	0.5708	$^1/_4$		
O18	6*h*	*m*..	0.333	0.3198	$^1/_4$		single atom P
(OH)19	6*h*	*m*..	0.3444	0.161	$^1/_4$		non-coplanar triangle Mo_3
M20	6*h*	*m*..	0.4435	0.2982	$^1/_4$		octahedron $(OH)_2O_4$
P21	6*h*	*m*..	0.4614	0.0426	$^1/_4$		trigonal bipyramid $(OH_2)O_4$
$(OH_2)22$	6*h*	*m*..	0.4955	0.1335	$^1/_4$	0.773	trigonal bipyramid $PO_3(OH)$
(OH)23	6*h*	*m*..	0.5383	0.2688	$^1/_4$		non-colinear $Mo(OH_2)$
O24	6*h*	*m*..	0.5673	0.0918	$^1/_4$		coplanar triangle $P(OH_2)Mo$
O25	4*f*	3..	$^1/_3$	$^2/_3$	0.0916	0.5	single atom P
P26	4*f*	3..	$^1/_3$	$^2/_3$	0.2232	0.5	
$(OH_2)27$	2*b*	-3..	0	0	0	0.773	square antiprism $(OH_2)_2O_6$
$(OH_2)28$	2*a*	-6..	0	0	$^1/_4$	0.773	8-vertex polyhedron $O_6(OH_2)_2$

M14 = 0.5Mo + 0.5V; M20 = 0.5Mo + 0.5V
Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.057

Remarks: Partial site occupancies are omitted in [1]; the authors state that the occupancies of the H_2O sites were fixed to give 8.5 molecules per formula unit. We assigned an approximate value to the occupancy of sites (OH_2) assuming statistical disorder. Short interatomic distances: d(P21-(OH_2)22) = 0.132 nm (in addition to a complete PO_4 tetrahedron), d(Rb3-(OH_2)1) = 0.138 nm. Short interatomic distances for partly occupied site(s). Ambiguous data: according to the chemical formula the core contains 9 OH, however, the authors state that part of M are bonded to terminal H_2O; we tentatively assigned OH to former site O16. Space group (173) $P6_3$ was tested and rejected. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Soghomonian V., Meyer L.A., Haushalter R.C., Zubieta J. (1998), Inorg. Chim. Acta 275/276, 122-129.