$V_3(V_{0.5}Mo_{0.5})_{39}Mo_{42}P_{49}$	*hP*133	(174) *P*-6 – $k^{22}j^{22}a$

$(V,Mo)_{84}P_{49}$ [1]

Structural features: $P(Mo,V)_6(Mo,V)_2$ bicapped and $P(Mo,V)_6(Mo,V)_3$ tricapped trigonal prisms (partial order Mo/V ignored) share atoms to form a 3D-framework with WC-type columns (3 P-centered prisms in the triangular cross-section).

Lomnytska Y.F. et al. (2004) [1]

$Mo_{61.50}P_{49}V_{22.50}$

$a = 2.52015$, $c = 0.33007$ nm, $c/a = 0.131$, $V = 1.8155$ nm^3, $Z = 1$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Mo1	3*k*	*m*..	0.00886	0.17555	$^1/_2$		monocapped trigonal prism P_5V_2
Mo2	3*k*	*m*..	0.01857	0.55789	$^1/_2$		square pyramid P_5
M3	3*k*	*m*..	0.08448	0.05386	$^1/_2$		monocapped square prism P_5V_4
M4	3*k*	*m*..	0.08894	0.46	$^1/_2$		monocapped square prism P_5V_4
M5	3*k*	*m*..	0.10905	0.34329	$^1/_2$		monocapped square prism P_5V_4
P6	3*k*	*m*..	0.11127	0.17243	$^1/_2$		trigonal prism V_2Mo_4
Mo7	3*k*	*m*..	0.15403	0.60625	$^1/_2$		monocapped trigonal prism P_5V_2
P8	3*k*	*m*..	0.19887	0.31443	$^1/_2$		square antiprism V_2Mo_6
M9	3*k*	*m*..	0.22648	0.48063	$^1/_2$		monocapped square prism P_5V_4
Mo10	3*k*	*m*..	0.25205	0.12533	$^1/_2$		square pyramid P_5
P11	3*k*	*m*..	0.25427	0.60013	$^1/_2$		square antiprism V_2Mo_6
P12	3*k*	*m*..	0.26057	0.22413	$^1/_2$		square antiprism Mo_7V
Mo13	3*k*	*m*..	0.30183	0.03778	$^1/_2$		monocapped trigonal prism P_5V_2
Mo14	3*k*	*m*..	0.30562	0.41289	$^1/_2$		monocapped trigonal prism P_5V_2
M15	3*k*	*m*..	0.35997	0.32573	$^1/_2$		tetrahedron P_4
M16	3*k*	*m*..	0.38757	0.17453	$^1/_2$		tetrahedron P_4
P17	3*k*	*m*..	0.39807	0.02833	$^1/_2$		square antiprism V_2Mo_6
P18	3*k*	*m*..	0.42977	0.28613	$^1/_2$		tricapped trigonal prism V_3Mo_6
P19	3*k*	*m*..	0.48887	0.17953	$^1/_2$		square antiprism Mo_7V
M20	3*k*	*m*..	0.54127	0.35443	$^1/_2$		tetrahedron P_4
P21	3*k*	*m*..	0.54647	0.08183	$^1/_2$		square antiprism Mo_7V
Mo22	3*k*	*m*..	0.59109	0.27	$^1/_2$		square pyramid P_5
M23	3*j*	*m*..	0.03027	0.36013	0		tetrahedron P_4
P24	3*j*	*m*..	0.03277	0.26113	0		square antiprism Mo_7V
M25	3*j*	*m*..	0.04057	0.11093	0		tetrahedron P_4
P26	3*j*	*m*..	0.08047	0.53693	0		square antiprism Mo_7V
Mo27	3*j*	*m*..	0.12434	0.2489	0		square pyramid P_5
P28	3*j*	*m*..	0.14187	0.42773	0		tricapped trigonal prism V_3Mo_6
P29	3*j*	*m*..	0.16897	0.06403	0		square antiprism Mo_7V
Mo30	3*j*	*m*..	0.17581	0.16316	0		square pyramid P_5
M31	3*j*	*m*..	0.18277	0.53843	0		tetrahedron P_4
V32	3*j*	*m*..	0.21017	0.38613	0		tetrahedron P_4
Mo33	3*j*	*m*..	0.26093	0.29797	0		monocapped trigonal prism P_5V_2
P34	3*j*	*m*..	0.30877	0.48713	0		square antiprism Mo_7V
P35	3*j*	*m*..	0.31647	0.11703	0		square antiprism V_2Mo_6
Mo36	3*j*	*m*..	0.32127	0.59099	0		square pyramid P_5
M37	3*j*	*m*..	0.34447	0.23333	0		monocapped square prism P_5V_4
P38	3*j*	*m*..	0.37057	0.39823	0		square antiprism Mo_6V_2
Mo39	3*j*	*m*..	0.4155	0.10722	0		monocapped trigonal prism P_5V_2
M40	3*j*	*m*..	0.46237	0.37113	0		monocapped square prism P_5V_4
Mo41	3*j*	*m*..	0.46305	0.01918	0		square pyramid P_5

M42	3*j*	*m*..	0.48237	0.25323	0	monocapped square prism P_5V_4
Mo43	3*j*	*m*..	0.54976	0.1548	0	monocapped trigonal prism P_5V_2
P44	3*j*	*m*..	0.59877	0.34463	0	square antiprism V_2Mo_6
P45	1*a*	-6..	0	0	0	tricapped trigonal prism V_3Mo_6

M3 = 0.78Mo + 0.22V; M4 = 0.72Mo + 0.28V; M5 = 0.68Mo + 0.32V; M9 = 0.72Mo + 0.28V; M15 = 0.72V + 0.28Mo; M16 = 0.61V + 0.39Mo; M20 = 0.77V + 0.23Mo; M23 = 0.71V + 0.29Mo; M25 = 0.65V + 0.35Mo; M31 = 0.67V + 0.33Mo; M37 = 0.68Mo + 0.32V; M40 = 0.53Mo + 0.47V; M42 = 0.52Mo + 0.48V
Transformation from published data: origin shift $^1/_3$ $^2/_3$ $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.054

References: [1] Lomnytska Y.F., Guérin R., Oryshchyn S.V., Kuz'ma Y.B., Babizhetskii V.S. (2004), Inorg. Mater. 40, 700-706 (Neorg. Mater. 40, 804-810).