$Ti(Ti_{0.45}Mo_{0.55})_8Mo_3P_7$	*hP*58	(174) *P*-6 – k^9j^9ecba

$(Ti,Mo)_{12}P_7$ [1]

Structural features: Infinite columns of base-linked $P(Mo,Ti)_6(Mo,Ti)_2$ bicapped and $P(Mo,Ti)_6(Mo,Ti)_3$ tricapped trigonal prisms (partial order Mo/Ti ignored) share atoms to form a 3D-framework with WC-type columns (3 P-centered prisms in the triangular cross-section); additional P in channels of hexagonal cross-section parallel to [001] (partial disorder).

Lomnytska Y.F. et al. (2003) [1]

$Mo_{8.24}P_{7.01}Ti_{3.76}$

a = 1.67821, c = 0.33196 nm, c/a = 0.198, V = 0.8097 nm^3, Z = 3

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
M1	3*k*	*m*..	0.0767	0.1685	$^1/_2$		tetrahedron P_4
M2	3*k*	*m*..	0.1164	0.368	$^1/_2$		15-vertex Frank-Kasper P_5Mo_9Ti
M3	3*k*	*m*..	0.1971	0.5901	$^1/_2$		7-capped pentagonal prism $P_5Mo_8Ti_4$
P4	3*k*	*m*..	0.2478	0.2047	$^1/_2$		square antiprism Ti_2Mo_6
M5	3*k*	*m*..	0.2917	0.0808	$^1/_2$		15-vertex Frank-Kasper $P_5Ti_3Mo_7$
P6	3*k*	*m*..	0.2959	0.4193	$^1/_2$		icosahedron Mo_7TiP_4
M7	3*k*	*m*..	0.4459	0.0387	$^1/_2$		7-capped pentagonal prism $P_7Mo_8Ti_2$
P8	3*k*	*m*..	0.4594	0.3758	$^1/_2$		square antiprism Mo_7Ti
M9	3*k*	*m*..	0.5322	0.2598	$^1/_2$		monocapped square prism P_5Mo_4
P10	3*j*	*m*..	0.0385	0.2442	0		square antiprism Mo_7Ti
Mo11	3*j*	*m*..	0.0389	0.5827	0		15-vertex Frank-Kasper $P_5Mo_8Ti_2$
P12	3*j*	*m*..	0.0915	0.4639	0		square antiprism Mo_6Ti_2
Ti13	3*j*	*m*..	0.1593	0.0871	0		16-vertex Frank-Kasper $P_6Mo_8Ti_2$
Mo14	3*j*	*m*..	0.2187	0.2965	0		15-vertex Frank-Kasper P_5Mo_9Ti
M15	3*j*	*m*..	0.2569	0.4949	0		14-vertex Frank-Kasper $P_4Mo_6Ti_4$
Mo16	3*j*	*m*..	0.3761	0.2555	0		15-vertex Frank-Kasper $P_5Mo_7Ti_3$
P17	3*j*	*m*..	0.4205	0.133	0		square antiprism Mo_6Ti_2
M18	3*j*	*m*..	0.5871	0.1612	0		14-vertex Frank-Kasper $P_4Mo_6Ti_4$
P19	1*e*	-6..	$^2/_3$	$^1/_3$	0		tricapped trigonal prism Mo_3Ti_6
P20	1*c*	-6..	$^1/_3$	$^2/_3$	0		tricapped trigonal prism Mo_3Ti_6
P21	1*b*	-6..	0	0	$^1/_2$	0.5	colinear P_2
P22	1*a*	-6..	0	0	0	0.52	colinear P_2

M1 = 0.51Mo + 0.49Ti; M2 = 0.83Mo + 0.17Ti; M3 = 0.65Ti + 0.35Mo; M5 = 0.81Mo + 0.19Ti; M7 = 0.79Mo + 0.21Ti; M9 = 0.65Ti + 0.35Mo; M15 = 0.76Mo + 0.24Ti; M18 = 0.84Mo + 0.16Ti

Transformation from published data: origin shift 0 0 $^1/_2$

Experimental: single crystal, diffractometer, X-rays, R = 0.073

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

References: [1] Lomnytska Y.F., Oryshchyn S.V., Babizhets'kii V.S., Kuz'ma Y.B. (2003), Inorg. Mater. 39, 555-561 (Neorg. Mater. 39, 664-670).