$(Ti_{0.75}Mo_{0.25})_6Mo_{5.3}P_7$	*hP*21	(174) *P*-6 – k^3j^3eda

$Ti_{4.5}Mo_{6.8}P_7$ [1]
Structural features: Infinite columns of base-linked $P[(Ti,Mo)_2Mo_4][(Ti,Mo)Mo]$ bicapped trigonal prisms ($P[(Ti,Mo)_3Mo_5]$ square antiprisms) and $P(Ti,Mo)_6(Ti,Mo)_3$ tricapped trigonal prisms share atoms to form a $Cr_{12}P_7$-type framework (sites with occ. < 0.15 and partial vacancies ignored); partial replacement of Mo_3 triangles by single Ti atoms (disorder).

Lomnytska Y.F. et al. (2001) [1]
$Mo_{6.81}P_7Ti_{4.52}$
a = 0.96835, c = 0.33091 nm, c/a = 0.342, V = 0.2687 nm^3, Z = 1

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
P1	3*k*	*m*..	0.19967	0.17333	$^1/_2$		10-vertex polyhedron Mo_5Ti_5
Mo2	3*k*	*m*..	0.29527	0.45963	$^1/_2$	0.84	single atom Ti
M3	3*k*	*m*..	0.44257	0.10093	$^1/_2$		non-colinear P_2
Mo4	3*j*	*m*..	0.03647	0.19913	0	0.85	single atom Ti
P5	3*j*	*m*..	0.10167	0.51433	0		10-vertex polyhedron Mo_5Ti_5
M6	3*j*	*m*..	0.40677	0.31713	0		tetrahedron P_4
P7	1*e*	-6..	$^2/_3$	$^1/_3$	0		tricapped trigonal prism Ti_9
Ti8	1*d*	-6..	$^1/_3$	$^2/_3$	$^1/_2$	0.12	tricapped trigonal prism Mo_3P_6
Ti9	1*a*	-6..	0	0	0	0.14	tricapped trigonal prism Mo_3P_6

M3 = 0.69Ti + 0.31Mo; M6 = 0.73Ti + 0.27Mo
Transformation from published data: *-y*,*-x*,*-z*; origin shift $^1/_3$ $^2/_3$ 0
Experimental: powder, diffractometer, X-rays, R = 0.092

Remarks: Homogeneity range $Ti_{11.3-x}Mo_xP_7$, 4.2 < x < 6.8. Short interatomic distances for partly occupied site(s). Space group (176) $P6_3/m$ was tested and rejected (R = 0.12).

References: [1] Lomnytska Y.F., Chykhrii S.I., Kuz'ma Y.B. (2001), J. Alloys Compd. 321, 91-96.