Ti_2P	*hP*81	(189) *P*-62*m* – $k^6j^3g^3f^5ca$

Ti_2P [1]
Structural features: Infinite columns of base-linked PTi_6Ti_3 tricapped trigonal prisms share atoms to form a 3D-framework (a framework of base- and edge-linked PTi_6 trigonal prisms with single prism columns shifted by *c*/2 in channels). Deformation derivative of Fe_2P.

Gemmi M. et al. (2003) [1]
PTi_2
a = 1.9969, c = 0.34589 nm, c/a = 0.173, V = 1.1945 nm^3, Z = 27

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Ti1	6*k*	*m*..	0.09	0.335	$^1/_2$		rhombic dodecahedron P_4Ti_{10}
P2	6*k*	*m*..	0.108	0.225	$^1/_2$		tricapped trigonal prism Ti_9
P3	6*k*	*m*..	0.108	0.558	$^1/_2$		tricapped trigonal prism Ti_9
P4	6*k*	*m*..	0.214	0.444	$^1/_2$		tricapped trigonal prism Ti_9
Ti5	6*k*	*m*..	0.245	0.576	$^1/_2$		14-vertex Frank-Kasper P_4Ti_{10}
Ti6	6*k*	*m*..	0.334	0.427	$^1/_2$		14-vertex Frank-Kasper P_4Ti_{10}
Ti7	6*j*	*m*..	0.122	0.455	0		7-capped pentagonal prism P_5Ti_{12}
Ti8	6*j*	*m*..	0.197	0.33	0		7-capped pentagonal prism P_5Ti_{12}
Ti9	6*j*	*m*..	0.33	0.53	0		pseudo Frank-Kasper P_6Ti_{12}
Ti10	3*g*	*m*2*m*	0.098	0	$^1/_2$		14-vertex Frank-Kasper P_4Ti_{10}
Ti11	3*g*	*m*2*m*	0.41	0	$^1/_2$		cuboctahedron P_4Ti_8
Ti12	3*g*	*m*2*m*	0.761	0	$^1/_2$		rhombic dodecahedron P_4Ti_{10}
Ti13	3*f*	*m*2*m*	0.206	0	0		7-capped pentagonal prism P_5Ti_{12}
P14	3*f*	*m*2*m*	0.33	0	0		tricapped trigonal prism Ti_9
Ti15	3*f*	*m*2*m*	0.528	0	0		pseudo Frank-Kasper P_6Ti_{12}
P16	3*f*	*m*2*m*	0.67	0	0		tricapped trigonal prism Ti_9
Ti17	3*f*	*m*2*m*	0.864	0	0		pseudo Frank-Kasper $Ti_{12}P_6$
P18	2*c*	-6..	$^1/_3$	$^2/_3$	0		tricapped trigonal prism Ti_9
P19	1*a*	-62*m*	0	0	0		tricapped trigonal prism Ti_9

Transformation from published data: -*x*,-*y*,-*z*
Experimental: polycrystalline sample, electron diffraction, R = 0.360

Remarks: Supersedes a report on Ti_2P with a smaller supercell (a = $\sqrt{3}$a(Fe_2P)) in [2].

References: [1] Gemmi M., Zou X.D., Hovmöller S., Migliori A., Vennström M., Andersson Y. (2003), Acta Crystallogr. A 59, 117-126. [2] Lundström T., Snell P.O. (1967), Acta Chem. Scand. 21, 1343-1352.