$[H_3O]_3Ti_6[PO_4]_7O_3[H_2O]_4$	*hP*112	(176) $P6_3/m$ – $i^3h^{11}f^2b$

$(H_3O)_3Ti_6(PO_4)_7O_3{\cdot}4H_2O$ [1]
Structural features: TiO_6 and $Ti(O_5[OH_2])$ octahedra and PO_4 tetrahedra (in part orientational disorder up-down) share vertices to form a 3D-framework; H_2O in large channels parallel to [001], H_3O in other channels.

Serre C., Férey G. (1999) [1]
$H_{17}O_{38}P_7Ti_6$
a = 1.59562, c = 0.6299 nm, c/a = 0.395, V = 1.3889 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*i*	1	0.2934	0.1023	0.0576		non-colinear PTi
O2	12*i*	1	0.4732	0.3633	0.0565		non-colinear PTi
O3	12*i*	1	0.5166	0.2044	0.1699	0.5	
O4	6*h*	*m*..	0.0304	0.5308	$^1/_4$		non-colinear PTi
O5	6*h*	*m*..	0.0489	0.2263	$^1/_4$		non-colinear PTi
Ti6	6*h*	*m*..	0.1128	0.4751	$^1/_4$		octahedron O_6
O7	6*h*	*m*..	0.1635	0.1559	$^1/_4$		single atom Ti
O8	6*h*	*m*..	0.1891	0.4135	$^1/_4$		non-colinear Ti_2
Ti9	6*h*	*m*..	0.1898	0.3042	$^1/_4$		octahedron O_6
O10	6*h*	*m*..	0.2297	0.6008	$^1/_4$		non-colinear P_2
P11	6*h*	*m*..	0.2791	0.0381	$^1/_4$		tetrahedron O_4
O12	6*h*	*m*..	0.3236	0.3377	$^1/_4$		non-colinear PTi
O13	6*h*	*m*..	0.3554	0.0068	$^1/_4$		non-colinear PTi
P14	6*h*	*m*..	0.4335	0.392	$^1/_4$		tetrahedron O_4
P15	4*f*	3..	$^1/_3$	$^2/_3$	0.1755	0.5	
O16	4*f*	3..	$^1/_3$	$^2/_3$	0.562	0.5	single atom P
(OH_2)17	2*b*	-3..	0	0	0		octahedron O_6
H18	12*i*	1	0.472	0.246	0.164	0.5	
H19	6*h*	*m*..	0.117	0.114	$^1/_4$		
H20	6*h*	*m*..	0.209	0.152	$^1/_4$		
H21	6*h*	*m*..	0.472	0.13	$^1/_4$		
H22	6*h*	*m*..	0.587	0.251	$^1/_4$		

Experimental: single crystal, diffractometer, X-rays, R = 0.039, T = 296 K

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Serre C., Férey G. (1999), C. R. Acad. Sci., Ser. IIc 2, 85-91.