



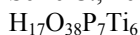
*hP*112

(176)  $P6_3/m - i^3h^{11}f^2b$

**(H<sub>3</sub>O)<sub>3</sub>Ti<sub>6</sub>(PO<sub>4</sub>)<sub>7</sub>O<sub>3</sub>·4H<sub>2</sub>O** [1]

Structural features: TiO<sub>6</sub> and Ti(O<sub>5</sub>[OH<sub>2</sub>]) octahedra and PO<sub>4</sub> tetrahedra (in part orientational disorder up-down) share vertices to form a 3D-framework; H<sub>2</sub>O in large channels parallel to [001], H<sub>3</sub>O in other channels.

Serre C., Férey G. (1999) [1]



$a = 1.59562$ ,  $c = 0.6299$  nm,  $c/a = 0.395$ ,  $V = 1.3889$  nm<sup>3</sup>,  $Z = 2$

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

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.