

$\text{Ca}_5[\text{PO}_4]_3\text{Cl}_{0.5}[\text{OH}]_{0.5}$ *hP*54 $(176) P6_3/m - \text{ih}^5\text{fe}^2$ **Ca<sub>5</sub>(PO<sub>4</sub>)<sub>3</sub>(OH,Cl)** [1], apatite family

Structural features: Infinite columns of base-linked CaO<sub>6</sub>O<sub>3</sub> tricapped trigonal prisms share atoms with PO<sub>4</sub> tetrahedra to form a 3D-framework; Cl and OH in infinite columns of face-linked Ca<sub>6</sub> octahedra (split site) parallel to [001] (partial disorder).

Sudarsanan K., Young R.A. (1978) [1]

 $\text{Ca}_{4.94}\text{Cl}_{0.59}\text{H}_{0.50}\text{O}_{12.50}\text{P}_3$  $a = 0.9564$ ,  $c = 0.6816$  nm,  $c/a = 0.713$ ,  $V = 0.5399$  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	0.0873	0.3513	0.068		single atom P
P2	6 <i>h</i>	<i>m</i> ..	0.0319	0.4041	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
O3	6 <i>h</i>	<i>m</i> ..	0.1251	0.5904	<sup>1</sup> / <sub>4</sub>		single atom P
Ca4	6 <i>h</i>	<i>m</i> ..	0.2462	0.2458	<sup>1</sup> / <sub>4</sub>	0.445	
Ca5	6 <i>h</i>	<i>m</i> ..	0.2656	0.2627	<sup>1</sup> / <sub>4</sub>	0.534	
O6	6 <i>h</i>	<i>m</i> ..	0.4887	0.1512	<sup>1</sup> / <sub>4</sub>		single atom P
Ca7	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0		trigonal prism O <sub>6</sub>
Cl8	4 <i>e</i>	3..	0	0	0.0791	0.294	
(OH)9	4 <i>e</i>	3..	0	0	0.1767	0.251	

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.058

Remarks: Natural specimen from Bluffton, Ohio. Refinement of the site occupancies showed no significant deviation from unity except for sites Ca4, Ca5, Cl8 and (OH)9. We took coordinates for site Ca7 from the literature, assuming  $z(\text{Ca7}) = 0$ . 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] Sudarsanan K., Young R.A. (1978), Acta Crystallogr. B 34, 1401-1407.