

$\text{Ca}_5[\text{PO}_4]_3\text{Cl}_{0.3}[\text{OH}]_{0.4}\text{F}_{0.3}$ *hP*56 $(176) P6_3/m - ih^5fe^2a$ **Ca₅(PO₄)₃(OH,Cl,F)** [1], apatite family

Structural features: Infinite columns of base-linked CaO₆O₃ tricapped trigonal prisms share atoms with PO₄ tetrahedra to form a 3D-framework; OH, Cl and F (partial disorder) in infinite columns of face-linked Ca₆ octahedra (split site) in channels parallel to [001].

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

 $\text{Ca}_{4.87}\text{Cl}_{0.34}\text{F}_{0.29}\text{H}_{0.41}\text{O}_{12.41}\text{P}_3$ $a = 0.9483$, $c = 0.678$ nm, $c/a = 0.715$, $V = 0.5280$ nm³, $Z = 2$

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	¹ / ₄		tetrahedron O ₄
O3	6 <i>h</i>	<i>m</i> ..	0.1251	0.5904	¹ / ₄		single atom P
Ca4	6 <i>h</i>	<i>m</i> ..	0.2464	0.2425	¹ / ₄	0.629	
Ca5	6 <i>h</i>	<i>m</i> ..	0.2705	0.2646	¹ / ₄	0.328	
O6	6 <i>h</i>	<i>m</i> ..	0.4887	0.1512	¹ / ₄		single atom P
Ca7	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0		trigonal prism O ₆
Cl8	4 <i>e</i>	3..	0	0	0.0928	0.17	
(OH)9	4 <i>e</i>	3..	0	0	0.1891	0.206	
F10	2 <i>a</i>	-6..	0	0	¹ / ₄	0.289	

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.034

Remarks: Natural specimen from Metale, Sri Lanka. Composition Ca_{9.93}(PO₄)_{5.81}(CO₃)_{0.27}(OH)_{0.76}F_{0.56}Cl_{0.66} from chemical analysis. We took the coordinates of site Ca7 from the literature, assuming $z(\text{Ca}7) = 0$, and those of the PO₄ units from the refinement of sample A in the same paper. 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.