

$\text{Ca}_5[\text{PO}_4]_3\text{Cl}_{0.3}[\text{OH}]_{0.3}\text{F}_{0.4}$
hP60

(176) $P6_3/m - ih^5fe^3a$
Ca₅(PO₄)₃(OH,Cl,F) [1], apatite family

Structural features: Infinite columns of base-linked CaO₆ trigonal prisms share vertices with PO₄ tetrahedra to form a 3D-framework; Cl, OH and F (the latter in trigonal coordination) in infinite columns of face-linked Ca₆ octahedra (split site) parallel to [001] (partial disorder).

Hughes J.M. et al. (1990) [1]

 $\text{Ca}_5\text{Cl}_{0.32}\text{F}_{0.40}\text{H}_{0.30}\text{O}_{12.30}\text{P}_3$
 $a = 0.94615$, $c = 0.68491$ nm, $c/a = 0.724$, $V = 0.5310$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.345	0.0853	0.0699		single atom P
O2	6 <i>h</i>	<i>m</i> ..	0.1547	0.4862	¹ / ₄		single atom P
Ca3	6 <i>h</i>	<i>m</i> ..	0.23861	0.2456	¹ / ₄	0.89	
Ca4	6 <i>h</i>	<i>m</i> ..	0.2709	0.2727	¹ / ₄	0.11	
P5	6 <i>h</i>	<i>m</i> ..	0.40053	0.03085	¹ / ₄		tetrahedron O ₄
O6	6 <i>h</i>	<i>m</i> ..	0.5884	0.1233	¹ / ₄		single atom P
Ca7	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0018		trigonal prism O ₆
Cl8	4 <i>e</i>	3..	0	0	0.06	0.08	
Cl9	4 <i>e</i>	3..	0	0	0.132	0.08	
(OH)10	4 <i>e</i>	3..	0	0	0.2	0.15	
F11	2 <i>a</i>	-6..	0	0	¹ / ₄	0.4	

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

Experimental: single crystal, diffractometer, X-rays, R = 0.015

Remarks: Natural specimen from Jackson Peek, Utah. Composition (Ca_{4.96}Mn_{0.01}Fe_{0.02}Sr_{0.01}Na_{0.02}Ce_{0.01})₅(P_{2.94}Si_{0.02}S_{0.02})O₁₂(F_{0.39}Cl_{0.33}OH_{0.28}) from electron microprobe analysis. 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] Hughes J.M., Cameron M., Crowley K.D. (1990), Am. Mineral. 75, 295-304.