

$\text{Ca}_5[\text{PO}_4]_3([\text{OH}]_{0.92}\text{F}_{0.08})$	<i>hP46</i>	(176) $P6_3/m - \text{ih}^4\text{fea}$
---	-------------	--

$\text{Ca}_5(\text{PO}_4)_3(\text{OH},\text{F})$ [1], hydroxylapatite, apatite family

Structural features: Infinite columns of base-linked CaO_6O_3 tricapped trigonal prisms share atoms with PO_4 tetrahedra to form a 3D-framework; OH and F in infinite columns of face-linked Ca_6 octahedra parallel to [001] (partial disorder).

Sudarsanan K., Young R.A. (1969) [1]

$\text{Ca}_5\text{F}_{0.08}\text{H}_{0.92}\text{O}_{12.92}\text{P}_3$

$a = 0.9424$, $c = 0.6879$ nm, $c/a = 0.730$, $V = 0.5291$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.3437	0.0858	0.0702		single atom P
O2	6 <i>h</i>	<i>m</i> ..	0.1564	0.4848	$\frac{1}{4}$		single atom P
Ca3	6 <i>h</i>	<i>m</i> ..	0.2468	0.2534	$\frac{1}{4}$		
P4	6 <i>h</i>	<i>m</i> ..	0.3987	0.0302	$\frac{1}{4}$		tetrahedron O ₄
O5	6 <i>h</i>	<i>m</i> ..	0.5873	0.1222	$\frac{1}{4}$		single atom P
Ca6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0015		trigonal prism O ₆
O7	4 <i>e</i>	3..	0	0	0.195	0.458	
F8	2 <i>a</i>	-6..	0	0	$\frac{1}{4}$	0.084	
H9	4 <i>e</i>	3..	0	0	0.0608	0.458	

Transformation from published data: *y,x,-z*

Experimental: single crystal, diffractometer, X-rays, R = 0.031

Remarks: Natural specimen from Holly Springs. 0.16-0.28 wt.% F found by chemical analysis, trace amounts of Mn and Mg. 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. (1969), Acta Crystallogr. B 25, 1534-1543.