

$\text{Ca}_5[\text{PO}_4]_3\text{F}$ $hP42$ $(176) P6_3/m - ih^4fa$

$\text{Ca}_5(\text{PO}_4)_3\text{F}$ [2], fluorapatite, apatite family, Strukturbericht notation H5₇; $\text{Ca}_5(\text{PO}_4)_3\text{OH}$ [4], hydroxylapatite

Structural features: Infinite columns of base-linked CaO_6O_3 tricapped trigonal prisms share atoms with PO_4 tetrahedra to form a 3D-framework; F (trigonal coordination) in infinite columns of face-linked Ca_6 octahedra parallel to [001]. See Fig. IV.67.

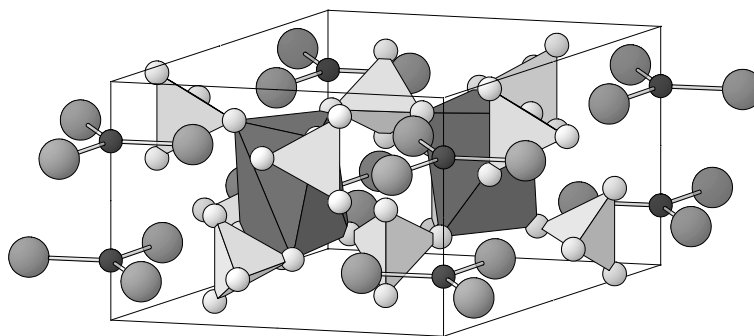


Fig. IV.67. **$\text{Ca}_5(\text{PO}_4)_3\text{F}$**

Arrangement of CaO_6 trigonal prisms (dark), PO_4 tetrahedra (light) (O atoms light) and FCa_3 triangles (F atoms dark, Ca atoms large).

Comodi P. et al. (2001) [1]

$\text{Ca}_5\text{FO}_{12}\text{P}_3$

$a = 0.9375$, $c = 0.6887$ nm, $c/a = 0.735$, $V = 0.5242$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.3416	0.0844	0.0705		single atom P
O2	6h	$m..$	0.1577	0.4844	$\frac{1}{4}$		single atom P
Ca3	6h	$m..$	0.24154	0.24875	$\frac{1}{4}$		pentagonal bipyramid FO_6
P4	6h	$m..$	0.39785	0.02932	$\frac{1}{4}$		tetrahedron O_4
O5	6h	$m..$	0.5873	0.1207	$\frac{1}{4}$		single atom P
Ca6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0011		tricapped trigonal prism O_9
F7	2a	-6..	0	0	$\frac{1}{4}$		coplanar triangle Ca_3

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.025$

Remarks: Strukturbericht notation H5₇ also refers to apatites with X in Wyckoff position 2b. The structure was determined independently in [3], where F was placed in Wyckoff position 2b. A refinement on powder X-ray diffraction data collected for ball-milled $\text{Ca}_5(\text{PO}_4)_3\text{F}$ is reported in [5].

References: [1] Comodi P., Liu Y., Zanazzi P.F., Montagnoli M. (2001), Phys. Chem. Miner. 28, 219-224. [2] Naray Szabo S. (1930), Z. Kristallogr. 75, 387-398. [3] Mehmeli M. (1930), Z. Kristallogr. 75, 323-331. [4] Hendricks S.B., Jefferson M.E., Mosley V.M. (1932), Z. Kristallogr. 81, 352-369. [5] Nikcevic I., Jokanovic V., Mitric M., Nedic Z., Makovec D., Uskokovic D. (2004), J. Solid State Chem. 177, 2565-2574.