$Ca_5[PO_4]_3[OH]$	*hP*44	(176) $P6_3/m$ – ih^{4}fe

$Ca_5(PO_4)_3OH$ [2], 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 (partial disorder) in infinite columns of face-linked Ca_6 octahedra in channels parallel to [001]. See Fig. IV.69.

Wilson R.M. et al. (1999) [1]
$Ca_5H_{0.16}O_{12.93}P_3$
a = 0.94081, c = 0.68887 nm, c/a = 0.732, V = 0.5280 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*i*	1	0.3417	0.0839	0.0711		single atom P
O2	6*h*	*m*..	0.1579	0.4849	$^1/_4$		single atom P
Ca3	6*h*	*m*..	0.2426	0.2522	$^1/_4$		
P4	6*h*	*m*..	0.3948	0.0291	$^1/_4$		tetrahedron O_4
O5	6*h*	*m*..	0.5791	0.1173	$^1/_4$		single atom P
Ca6	4*f*	3..	$^1/_3$	$^2/_3$	0.0007		tricapped trigonal prism O_9
O7	4*e*	3..	0	0	0.1837	0.465	
H8	4*e*	3..	0	0	0.0608	0.08	

Transformation from published data: *y*,*x*,-*z*
Experimental: powder, diffractometer, X-rays, wR_p = 0.095

Remarks: Short interatomic distances for partly occupied site(s). Refinement of the site occupancies showed no significant deviation from unity except for sites O7 and H8. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

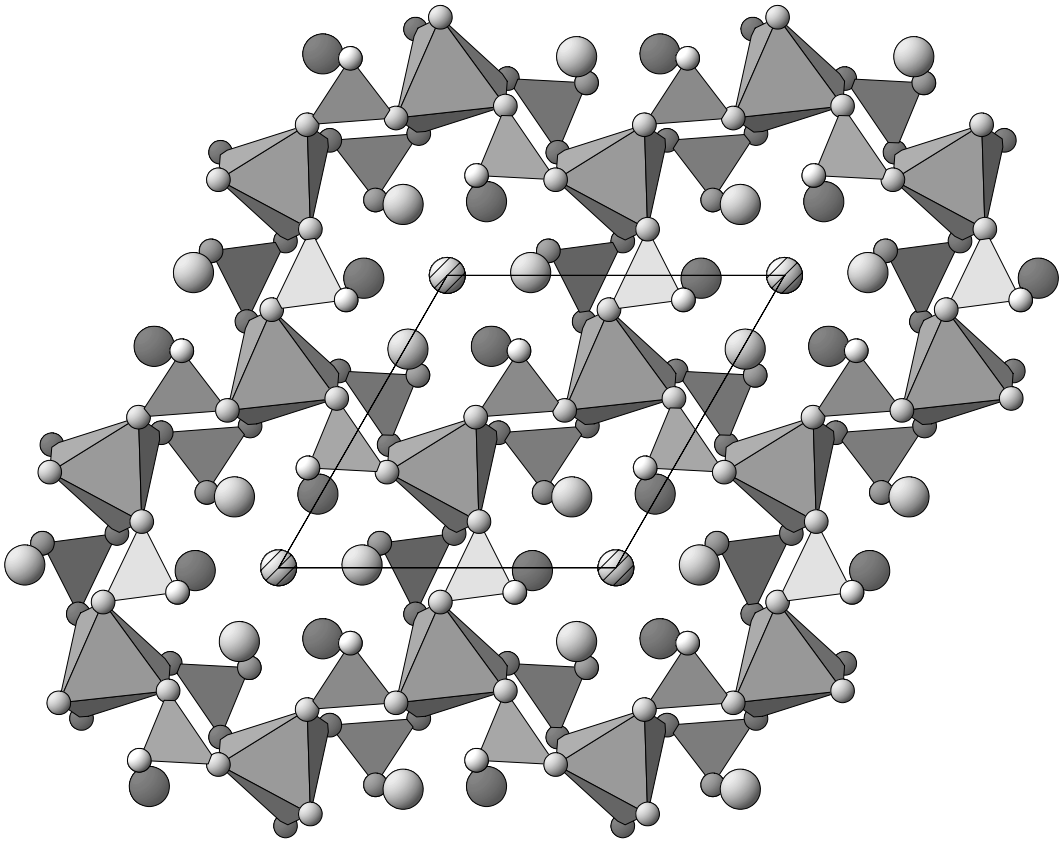

Fig. IV.69. **$Ca_5(PO_4)_3OH$** STP06777

Arrangement of CaO_6 trigonal prisms, PO_4 tetrahedra (O atoms small), additional Ca atoms (large) and OH units (O atoms medium; partly occupied site) viewed along [001]. Light and dark tetrahedra are shifted by *c*/2.

References: [1] Wilson R.M., Elliott J.C., Dowker S.E.P. (1999), Am. Mineral. 84, 1406-1414. [2] Kay M.I., Young R.A., Posner A.S. (1964), Nature (London) 204, 1050-1052.