$Ca_5[PO_4]_3Cl$	*hP*42	(176) $P6_3/m$ – ih^4fb

$Ca_5(PO_4)_3Cl$ [1], chlorapatite, apatite family, Strukturbericht notation $H5_7$; $Ba_5(PO_4)_3Cl$ [2], alforsite
Structural features: Infinite columns of base-linked CaO_6O_3 tricapped trigonal prisms share atoms with PO_4 tetrahedra to form a 3D-framework; infinite columns of face-linked $ClCa_6$ octahedra in channels parallel to [001]. See Fig. IV.68.

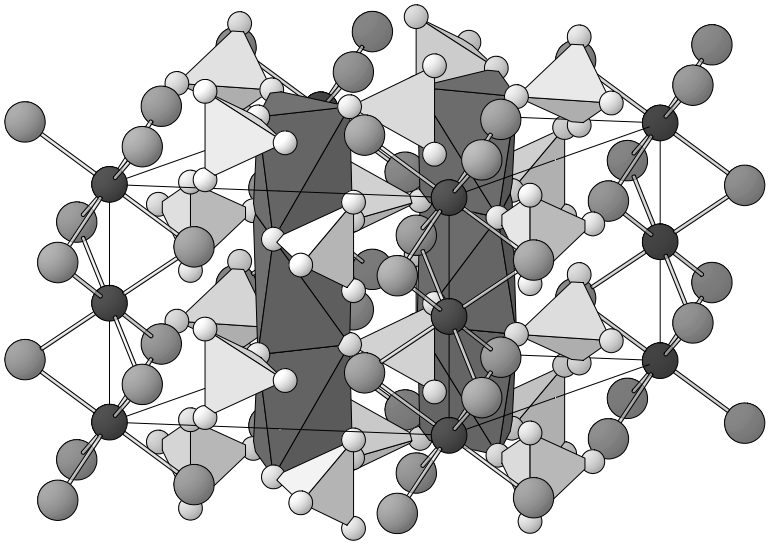

Fig. IV.68. **$Ca_5(PO_4)_3Cl$**

Arrangement of CaO_6 trigonal prisms (dark), PO_4 tetrahedra (light) (O atoms light) and $ClCa_6$ octahedra (Cl atoms dark, Ca atoms large).

Hendricks S.B. et al. (1932) [1]
$Ca_5ClO_{12}P_3$
$a = 0.952$, $c = 0.685$ nm, $c/a = 0.720$, $V = 0.5376$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	12*i*	1	0.083	0.333	0.064		single atom P
P2	6*h*	*m*..	0.055	0.416	$^1/_4$		tetrahedron O_4
O3	6*h*	*m*..	0.133	0.6	$^1/_4$		single atom P
Ca4	6*h*	*m*..	0.247	0.25	$^1/_4$		tricapped trigonal prism O_6Cl_2P
O5	6*h*	*m*..	0.5	0.167	$^1/_4$		single atom P
Ca6	4*f*	3..	$^1/_3$	$^2/_3$	0.0		trigonal prism O_6
Cl7	2*b*	-3..	0	0	0		icosahedron O_6Ca_6

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, Weissenberg photographs, X-rays

Remarks: Natural specimen from the Bamle mines, Kragerö, Norway. 52.97 wt.% CaO, 0.29 wt.% MgO, 40.50 wt.% P_2O_5, 0.17 wt.% F, 4.13 wt.% Cl, 0.22 wt.% Na_2O, 0.10 wt.% K_2O, 1.16 wt.% SiO_2, and 0.18 wt.% Fe_2O_3 found by chemical analysis. Strukturbericht notation $H5_7$ also refers to apatites with X in Wyckoff position 2*a*.

References: [1] Hendricks S.B., Jefferson M.E., Mosley V.M. (1932), Z. Kristallogr. 81, 352-369. [2] Hata M., Marumo F., Iwai S., Aoki H. (1979), Acta Crystallogr. B 35, 2382-2384.