$Ca_{4.7}Nd_{0.2}[PO_4]_3F$	*hP*48	(176) $P6_3/m$ – ih^{5}fa

$Ca_5(PO_4)_3F$:Nd [1], apatite family; $Na_3Ca_2(SO_4)_3OH$ rt [2], cesanite
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 (in trigonal coordination) in infinite columns of face-linked $(Ca,Nd)_6$ octahedra parallel to [001] (distinct positions for Ca and Nd).

Mackie P.E., Young R.A. (1973) [1]
$Ca_{4.09}F_{0.91}Nd_{0.24}O_{12}P_3$
a = 0.93674, c = 0.68837 nm, c/a = 0.735, V = 0.5231 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*i*	1	0.3419	0.0849	0.0704		single atom P
O2	6*h*	*m*..	0.1581	0.4846	$^1/_4$		single atom P
Nd3	6*h*	*m*..	0.2331	0.2425	$^1/_4$	0.08	
Ca4	6*h*	*m*..	0.2425	0.2492	$^1/_4$	0.716	
P5	6*h*	*m*..	0.3985	0.0294	$^1/_4$		tetrahedron O_4
O6	6*h*	*m*..	0.5883	0.1214	$^1/_4$		single atom P
Ca7	4*f*	3..	$^1/_3$	$^2/_3$	0.0011	0.973	trigonal prism O_6
F8	2*a*	-6..	0	0	$^1/_4$	0.906	

Transformation from published data: *y*,*x*,-*z*
Experimental: single crystal, diffractometer, X-rays, R = 0.013

Remarks: 18-34 % of the reflections were omitted from the refinement. Refinement of the occupancies of the O sites showed no significant deviation from unity; we set the occupancy of site P5 equal to unity (refined value 1.014(2)). Short interatomic distances for partly occupied site(s). The same Ca/Na ratio is reported for both parts of the split site in [2] (cesanite).

References: [1] Mackie P.E., Young R.A. (1973), J. Appl. Crystallogr. 6, 26-31. [2] Deganello S. (1983), Neues Jahrb. Mineral., Monatsh. 1983, 305-313.