$[NH_4]_{0.05}Ca_{4.65}[PO_4]_{2.48}[CO_3]_{0.54}[OH]_{0.83}[H_2O]_{0.38}$	*hP*68	(176) $P6_3/m$ – i^2h^6fe

$(NH_4)_{0.1}Ca_{9.5}(PO_4)_{5.05}(CO_3)_{0.95}(OH)_{2.05}$ [1], apatite family
Structural features: Infinite columns of base-linked CaO_6 trigonal prisms (partial vacancies ignored) share vertices with PO_4 tetrahedra and CO_3 trigonal units (substitutional disorder) to form a 3D-framework; OH in infinite columns of face-linked $(Ca,NH_4)_6$ octahedra parallel to [001] (partial disorder).

Ivanova T.I. et al. (2001) [1]
$C_{0.54}Ca_{4.65}H_{1.41}N_{0.05}O_{12.95}P_{2.47}$
a = 0.94372, c = 0.68881 nm, c/a = 0.73, V = 0.5313 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*i*	1	0.3409	0.083	0.0668	0.832	
O2	12*i*	1	0.362	0.063	0.089	0.187	
C3	6*h*	*m*..	0.0096	0.3618	$^1/_4$	0.09	
O4	6*h*	*m*..	0.1565	0.4829	$^1/_4$	0.932	
M5	6*h*	*m*..	0.2457	0.2578	$^1/_4$		
P6	6*h*	*m*..	0.3991	0.0299	$^1/_4$	0.824	
C7	6*h*	*m*..	0.438	0.083	$^1/_4$	0.09	
O8	6*h*	*m*..	0.5879	0.1184	$^1/_4$	0.945	
Ca9	4*f*	3..	$^1/_3$	$^2/_3$	0.0011	0.848	trigonal prism O_6
(OH)10	4*e*	3..	0	0	0.1884	0.602	

M5 = 0.983Ca + 0.017NH_4
Transformation from published data: *y*,*x*,-*z*
Experimental: powder, diffractometer, X-rays, R_p = 0.049, T = 298 K

Remarks: We adjusted the charge balance in the published chemical formula by changing the OH index from 2 to 2.05. $Ca_{3.4}[Ca_{5.9}(NH_4)_{0.1}][(PO_4)_{4.95}(CO_3)_{1.05}(H_2O)_{0.30}][(OH)_{1.65}(H_2O)_{0.45}]$ (neutral for OH index 1.75). Refinement considering f(Ca) for site M5 gave occ = 0.985(2). Short interatomic distances for partly occupied site(s); impossibly short distances occur for published site occupancies. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Ivanova T.I., Frank Kamenetskaya O.V., Kol'tsov A.B., Ugolkov V.L. (2001), J. Solid State Chem. 160, 340-349.