$H_{0.65}K_{0.17}Ca_{4.20}[PO_4]_{2.22}[CO_3]_{0.78}[OH]$	*hP*68	(176) $P6_3/m$ – i^3h^4fe

$K_{0.34}Ca_{8.40}(PO_4)_{3.15}(HPO_4)_{1.30}(CO_3)_{1.55}(OH)_2$ [1], apatite family
Structural features: Infinite columns of base-linked CaO_6O_3 tricapped trigonal prisms (partial vacancies ignored) share atoms with $P[O_3(O,OH)]$ tetrahedra and CO_3 trigonal units (substitutional disorder) to form a 3D-framework; OH in infinite columns of face-linked Ca octahedra (partial vacancies ignored) parallel to [001] (partial disorder).

Ivanova T.I. et al. (2004) [1]
$C_{0.75}Ca_{4.37}H_{1.80}O_{13.42}P_{2.25}$
a = 0.94015, c = 0.68985 nm, c/a = 0.734, V = 0.5281 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*i*	1	0.042	0.374	0.088	0.22	
O2	12*i*	1	0.1569	0.4865	0.234	0.506	
M3	12*i*	1	0.3407	0.085	0.0687	0.827	single atom O
Ca4	6*h*	*m*..	0.2462	0.2545	$^1/_4$	0.901	non-coplanar triangle O_3
M5	6*h*	*m*..	0.3992	0.03	$^1/_4$		non-coplanar triangle O_3
O6	6*h*	*m*..	0.535	0.16	$^1/_4$	0.25	
O7	6*h*	*m*..	0.5867	0.1204	$^1/_4$	0.765	
Ca8	4*f*	3..	$^1/_3$	$^2/_3$	0.0029	0.835	
(OH)9	4*e*	3..	0	0	0.169	0.528	single atom (OH)

M3 = 0.85O + 0.15OH; M5 = 0.75P + 0.25C
Transformation from published data: *y*,*x*,-*z*
Experimental: powder, diffractometer, X-rays, R_B = 0.023, T = 298 K

Remarks: No attempt was made to distinguish Ca and K in the refinement. Refinement of the occupancy of site M5 considering f(P) gave occ = 0.835(2). We assigned approximate values to the C/P ratio of site M5 and O/OH ratio of site M3 based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In the abstract of [1] the chemical formula is misprinted as $Ca_{8.40}K_{0.34}$_ $[(PO_4)_{3.15}(HPO_4)_{1.30}(CO_3)]_{1.55}(OH)_2$ instead of $Ca_{8.40}K_{0.34}[(PO_4)_{3.15}(HPO_4)_{1.30}(CO_3)_{1.55}](OH)_2$ (given on page 480). Distinct positions were considered for P and C in [2].

References: [1] Ivanova T.I., Frank Kamenetskaya O.V., Kol'tsov A.B. (2004), Z. Kristallogr. 219, 479-486. [2] Ivanova T.I., Frank Kamenetskaya O.V., Kol'tsov A.B., Ugolkov V.L. (2001), J. Solid State Chem. 160, 340-349.