$KCa_{1.1}Mg(Al_{0.29}Si_{0.71})_{18}O_{36}$	*hP*84	(187) *P*-6*m*2 – $o^3n^2ml^2kj^4eca$

$K_{1.04}Ca_{1.04}Mg_{0.95}Al_{5.2}Si_{12.8}O_{36}$ [1], offretite, zeolite OFF
Structural features: $(Si,Al)O_4$ tetrahedra share vertices to form an OFF-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, gmelinite-type cages (nine 4-rings, two planar 6-rings and three non-planar 8-rings), and channels delimited by 12-rings parallel to [001]; Ca at the centers of cancrinite-type cages, Mg at the centers of 6-rings, K at the centers of 8-rings. ERI-type stacking faults.

Mortier W.J. et al. (1976) [1]
$Al_{5.22}CaK_{1.03}Mg_{0.84}O_{36}Si_{12.78}$
a = 1.3229, c = 0.7338 nm, c/a = 0.555, V = 1.1121 nm^3, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*o*	1	0.0408	0.3511	0.1818	0.89	
M2	12*o*	1	0.2279	0.0002	0.2823		
O3	12*o*	1	0.343	0.041	0.188	0.11	
O4	6*n*	.*m*.	0.0896	0.9104	0.2216		non-colinear Si_2
O5	6*n*	.*m*.	0.8722	0.1278	0.2121		non-coplanar square Si_2O_2
O6	6*m*	*m*..	0.003	0.2483	$^1/_2$		non-colinear Si_2
M7	6*l*	*m*..	0.0968	0.4273	0	0.89	tetrahedron O_4
M8	6*l*	*m*..	0.432	0.099	0	0.11	tetrahedron O_4
K9	3*k*	*mm*2	0.4964	0.5036	$^1/_2$	0.345	
O10	3*j*	*mm*2	0.2425	0.7575	0	0.89	non-colinear Si_2
O11	3*j*	*mm*2	0.4592	0.5408	0	0.89	non-colinear Si_2
O12	3*j*	*mm*2	0.553	0.447	0	0.11	non-colinear Si_2
O13	3*j*	*mm*2	0.749	0.251	0	0.11	coplanar triangle Si_2Mg
Mg14	1*e*	-6*m*2	$^2/_3$	$^1/_3$	0	0.11	coplanar triangle O_3
Mg15	1*c*	-6*m*2	$^1/_3$	$^2/_3$	0	0.727	coplanar triangle O_3
Ca16	1*a*	-6*m*2	0	0	0		trigonal prism O_6

M2 = 0.71Si + 0.29Al; M7 = 0.71Si + 0.29Al; M8 = 0.71Si + 0.29Al
Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, wR = 0.033

Remarks: Natural specimen from Mt. Simiouse, France, dehydrated at 773 K in vacuum. We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition and set the occupancy of site Ca16 equal to unity (refined value 1.044(13)). Short interatomic distances for partly occupied site(s). In [1] the origin of the mineral is misprinted as Mt. Simionse instead of Mt. Simiouse.

References: [1] Mortier W.J., Pluth J.J., Smith J.V. (1976), Z. Kristallogr. 143, 319-332.