$KCa_{1.1}Mg(Al_{0.29}Si_{0.71})_{18}O_{36}[CO]$	*hP*89	(187) *P*-6*m*2 – $o^3n^2ml^2kj^4hg^2eb$

$K_{1.04}Ca_{1.04}Mg_{0.95}Al_{5.2}Si_{12.8}O_{36}\cdot CO$ [1], zeolite OFF (CO)
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, K at the centers of 8-rings, Mg above 6-rings, coordinated to CO. ERI-type stacking faults.

Mortier W.J. et al. (1976) [1]
$Al_{5.18}C_{0.88}CaKMg_{1.05}O_{36.70}Si_{12.76}$
a = 1.3261, c = 0.7347 nm, c/a = 0.554, V = 1.1189 nm^3, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*o*	1	0.00467	0.36133	0.17	0.087	
O2	12*o*	1	0.31407	0.02463	0.1824	0.903	
M3	12*o*	1	0.43917	0.10623	0.2821		trigonal bipyramid O_5
O4	6*n*	.*m*.	0.53837	0.46163	0.2108		non-colinear Si_2
O5	6*n*	.*m*.	0.75557	0.24443	0.2215		non-colinear Si_2
O6	6*m*	*m*..	0.41897	0.08923	$^1/_2$		non-colinear Si_2
M7	6*l*	*m*..	0.09567	0.43733	0	0.087	tetrahedron O_4
M8	6*l*	*m*..	0.23817	0.00233	0	0.903	tetrahedron O_4
K9	3*k*	*mm*2	0.15817	0.84183	$^1/_2$	0.334	
O10	3*j*	*mm*2	0.12667	0.87333	0	0.903	non-colinear Si_2
O11	3*j*	*mm*2	0.22267	0.77733	0	0.087	non-colinear Si_2
O12	3*j*	*mm*2	0.43267	0.56733	0	0.087	non-colinear Si_2
O13	3*j*	*mm*2	0.91117	0.08883	0	0.903	non-colinear Si_2
Mg14	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.03	0.087	
Mg15	2*g*	3*m*.	0	0	0.052	0.44	
C16	2*g*	3*m*.	0	0	0.346	0.44	single atom O
Ca17	1*e*	-6*m*2	$^2/_3$	$^1/_3$	0		trigonal prism O_6
O18	1*b*	-6*m*2	0	0	$^1/_2$	0.88	colinear C_2

M3 = 0.711Si + 0.289Al; M7 = 0.711Si + 0.289Al; M8 = 0.711Si + 0.289Al
Transformation from published data: origin shift $^1/_3$ $^2/_3$ $^1/_2$
Experimental: single crystal, diffractometer, X-rays, wR = 0.032

Remarks: Natural specimen from Mt. Simiouse, France; dehydrated and submitted to CO pressure. Short interatomic distances for partly occupied site(s). We assigned an approximate value to the Al/Si ratio of sites M based on the nominal composition. 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. 144, 32-41.