$K_{3.9}Na_{9.1}Ca_{11}Al_{18}[SiO_4]_{18}[SO_4]_5Cl_{3.5}F_{0.5}$	*hP*222	(174) *P*-6 – $l^{27}k^5j^8i^2h^4g^3fec$

$(Na,K)_{16}Ca_8Al_{18}Si_{18}O_{72}(SO_4)_5Cl_4$ [1], liottite, zeolite LIO

Structural features: AlO_4 and SiO_4 tetrahedra share vertices to form a LIO-type zeolite framework (6-rings in ABABAC stacking) with columns of base-linked cancrinite-type cages (six 4-rings and five 6-rings), columns of base-linked losod- (six 4-rings and eleven 6-rings) and cancrinite-type cages and columns of base-linked liottite-type cages (six 4-rings and seventeen 6-rings); Ca at and near the centers of 6-rings, Cl and F in cancrinite cages (partial disorder), SO_4 tetrahedra and (Na,K,Ca) in the larger cages.

Ballirano P. et al. (1996) [1]

$Al_{18}Ca_{7.98}Cl_{3.50}F_{0.50}K_{6.90}Na_{9.12}O_{92}S_5Si_{18}$

a = 1.287, c = 1.6096 nm, c/a = 1.251, V = 2.3089 nm^3, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6*l*	1	0.0014	0.344	0.2543		non-colinear SiAl
S2	6*l*	1	0.023	0.036	0.2874	0.167	
O3	6*l*	1	0.051	0.11	0.021	0.333	
O4	6*l*	1	0.054	0.119	0.345	0.333	non-colinear OS
O5	6*l*	1	0.058	0.119	0.074	0.333	
O6	6*l*	1	0.0582	0.1213	0.2676	0.667	single atom S
Al7	6*l*	1	0.0718	0.4149	0.16345		tetrahedron O_4
O8	6*l*	1	0.094	0.056	0.223	0.167	non-colinear SO
O9	6*l*	1	0.1097	0.5633	0.1545		non-colinear SiAl
M10	6*l*	1	0.1636	0.3358	0.3313	0.92	
M11	6*l*	1	0.184	0.375	0.347	0.08	
O12	6*l*	1	0.2067	0.4172	0.1632		non-colinear SiAl
M13	6*l*	1	0.2261	0.1136	0.1651	0.9	
O14	6*l*	1	0.269	0.5405	0.3789	0.667	
O15	6*l*	1	0.272	0.56	0.413	0.333	
M16	6*l*	1	0.294	0.149	0.175	0.1	
O17	6*l*	1	0.308	0.606	0.289	0.167	
O18	6*l*	1	0.3228	0.329	0.0856		non-colinear SiAl
O19	6*l*	1	0.3237	0.3294	0.4182		non-colinear SiAl
Si20	6*l*	1	0.32818	0.41035	0.16374		tetrahedron O_4
O21	6*l*	1	0.331	0.3463	0.2491		non-colinear SiAl
O22	6*l*	1	0.3341	0.0076	0.0794		non-colinear SiAl
O23	6*l*	1	0.3369	0.0067	0.4119		non-colinear SiAl
Al24	6*l*	1	0.4088	0.3339	0.33304		tetrahedron O_4
Si25	6*l*	1	0.41483	0.08094	0.33287		tetrahedron O_4
O26	6*l*	1	0.4293	0.2114	0.3253		non-colinear SiAl
O27	6*l*	1	0.5499	0.1051	0.3386		non-colinear SiAl
M28	3*k*	*m*..	0.1085	0.5542	$^1/_2$		non-colinear O_2
O29	3*k*	*m*..	0.1229	0.2487	$^1/_2$		non-colinear SiAl
O30	3*k*	*m*..	0.2227	0.1202	$^1/_2$		non-colinear SiAl
Si31	3*k*	*m*..	0.2517	0.2563	$^1/_2$		tetrahedron O_4
Al32	3*k*	*m*..	0.2622	0.011	$^1/_2$		tetrahedron O_4
S33	3*j*	*m*..	0.017	0.0357	0	0.333	
M34	3*j*	*m*..	0.143	0.286	0	0.25	
M35	3*j*	*m*..	0.1537	0.3188	0	0.75	
F36	3*j*	*m*..	0.2524	0.5224	0	0.167	single atom Cl
Al37	3*j*	*m*..	0.4097	0.3364	0		tetrahedron O_4
Si38	3*j*	*m*..	0.4127	0.0827	0		tetrahedron O_4

O39	3*j*	*m*..	0.4337	0.2164	0		non-colinear SiAl
O40	3*j*	*m*..	0.546	0.1017	0		non-colinear SiAl
Cl41	2*i*	3..	$^2/_3$	$^1/_3$	0.1665		colinear Ca_2
Ca42	2*i*	3..	$^2/_3$	$^1/_3$	0.333		hexagonal bipyramid O_6Cl_2
Ca43	2*h*	3..	$^1/_3$	$^2/_3$	0.1085	0.5	
Ca44	2*h*	3..	$^1/_3$	$^2/_3$	0.1564	0.5	
O45	2*h*	3..	$^1/_3$	$^2/_3$	0.2591	0.5	
S46	2*h*	3..	$^1/_3$	$^2/_3$	0.3568		
S47	2*g*	3..	0	0	0.2971	0.5	
O48	2*g*	3..	0	0	0.386	0.5	
Ca49	2*g*	3..	0	0	0.4783	0.5	
Cl50	1*f*	-6..	$^2/_3$	$^1/_3$	$^1/_2$		colinear Ca_2
Ca51	1*e*	-6..	$^2/_3$	$^1/_3$	0		hexagonal bipyramid O_6Cl_2
Cl52	1*c*	-6..	$^1/_3$	$^2/_3$	0	0.5	trigonal bipyramid F_3Ca_2

M10 = 0.59Na + 0.32K + 0.09Ca; M11 = 0.59Na + 0.32K + 0.09Ca; M13 = 0.44K + 0.43Na + 0.13Ca; M16 = 0.44K + 0.43Na + 0.13Ca; M28 = 0.45K + 0.42Na + 0.13Ca; M34 = 0.58Na + 0.33K + 0.09Ca; M35 = 0.58Na + 0.33K + 0.09Ca
Transformation from published data: *y*,*x*,*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.028

Remarks: Natural specimen from Pitigliano, Tuscany, Italy. Composition $(Na_{9.78}K_{4.68}Ca_{9.12})[Si_{18.24}Al_{17.76}O_{72.27}](SO_4)_{5.16}Cl_{3.39}F_{0.69}$ from electron microprobe analysis. No attempt was made to distinguish Ca and K in the refinement. We assigned an approximate value to the Ca/K ratio of sites M based on the chemical analysis. Short interatomic distances for partly occupied site(s). Space group (187) *P*-6*m*2 was tested (disorder Si/Al) and rejected (R = 0.066). The average structure was refined in space group (187) *P*-6*m*2 in [2].

References: [1] Ballirano P., Merlino S., Bonaccorsi E., Maras A. (1996), Can. Mineral. 34, 1021-1030. [2] Merlino S., Mellini M. (1976), Zeolites '76, Tuscon, 1976, Coll. Abstr. 47.