

$\text{K}_{1.1}\text{Ca}_{1.2}\text{Mg}_{0.7}(\text{Al}_{0.58}\text{Si}_{0.42})_9[\text{SiO}_4]_9[\text{H}_2\text{O}]_{15.2}$
hP88

(187) *P-6m2* – $\text{o}^2\text{n}^3\text{ml}^3\text{k}^3\text{j}^2\text{hgda}$
 $\text{K}_{1.1}\text{Ca}_{1.2}\text{Mg}_{0.7}\text{Al}_{5.2}\text{Si}_{12.8}\text{O}_{36}\cdot 15.2\text{H}_2\text{O}$ [1], offretite, zeolite OFF hydrated

Structural features: SiO_4 and $(\text{Si},\text{Al})\text{O}_4$ 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]; K at the centers of cancrinite-type cages, hydrated Mg at the centers of gmelinite-type cages, Ca and H_2O in the channels, additional Ca at the centers of 6-rings.

Gard J.A., Tait J.M. (1972) [1]

 $\text{Al}_{4.44}\text{Ca}_{0.92}\text{H}_{19.68}\text{KMg}_{0.82}\text{O}_{45.84}\text{Si}_{13.56}$
 $a = 1.3291$, $c = 0.7582$ nm, $c/a = 0.570$, $V = 1.1599$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>o</i>	1	0.01133	0.31567	0.329		non-colinear Si ₂
M2	12 <i>o</i>	1	0.10183	0.43247	0.2085		tetrahedron O ₄
O3	6 <i>n</i>	. <i>m</i> .	0.23233	0.76767	0.257		non-colinear Si ₂
O4	6 <i>n</i>	. <i>m</i> .	0.46033	0.53967	0.293		non-colinear Si ₂
(OH ₂)5	6 <i>n</i>	. <i>m</i> .	0.77133	0.22867	0.172	0.47	non-colinear (OH ₂) ₂
Si6	6 <i>m</i>	<i>m</i> ..	0.00123	0.24157	$\frac{1}{2}$		tetrahedron O ₄
O7	6 <i>l</i>	<i>m</i> ..	0.07833	0.39967	0		non-colinear Si ₂
(OH ₂)8	6 <i>l</i>	<i>m</i> ..	0.17333	0.02667	0	0.14	non-colinear (OH ₂) ₂
(OH ₂)9	6 <i>l</i>	<i>m</i> ..	0.51333	0.19667	0	0.17	non-coplanar triangle (OH ₂) ₃
O10	3 <i>k</i>	<i>mm2</i>	0.10333	0.89667	$\frac{1}{2}$		non-colinear Si ₂
(OH ₂)11	3 <i>k</i>	<i>mm2</i>	0.57533	0.42467	$\frac{1}{2}$	0.58	non-colinear Ca ₂
O12	3 <i>k</i>	<i>mm2</i>	0.87033	0.12967	$\frac{1}{2}$		non-colinear Si ₂
(OH ₂)13	3 <i>j</i>	<i>mm2</i>	0.09033	0.90967	0	0.34	non-colinear (OH ₂) ₂
(OH ₂)14	2 <i>i</i>	3 <i>m</i> .	$\frac{2}{3}$	$\frac{1}{3}$	0.24	0.3	
Ca15	2 <i>i</i>	3 <i>m</i> .	$\frac{2}{3}$	$\frac{1}{3}$	0.377	0.39	
Ca16	2 <i>h</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.13	0.07	
(OH ₂)17	2 <i>g</i>	3 <i>m</i> .	0	0	0.261	0.9	single atom Mg
K18	1 <i>d</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		bicapped hexagonal prism Ca ₂ O ₁₂
Mg19	1 <i>a</i>	-6 <i>m2</i>	0	0	0	0.82	

 $\text{M2} = 0.63\text{Si} + 0.37\text{Al}$

Transformation from published data: -*x*, -*y*, -*z*; origin shift $\frac{2}{3}$ $\frac{1}{3}$ 0

Experimental: single crystal, diffractometer, X-rays, R = 0.096

Remarks: Natural specimen from Mt. Simiouse, Monbrison, Loire, France. Composition $\text{K}_{1.1}\text{Ca}_{1.1}\text{Mg}_{0.7}\text{Al}_{5.2}\text{Si}_{12.8}\text{O}_{36}\cdot 15.2\text{H}_2\text{O}$ from chemical analysis. We adjusted the charge balance in the chemical formula given above by adding Ca. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Gard J.A., Tait J.M. (1972), Acta Crystallogr. B 28, 825-834.