

KCaMg(Al_{0.28}Si_{0.72})₁₈O₃₆[H₂O]₁₇

*hP*86

(187) *P-6m2* – o²n³ml³k³j²i²gda

KCaMgAl₅Si₁₃O₃₆·17H₂O [1], offretite, zeolite OFF hydrated

Structural features: (Si,Al)O₄ 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 additional H₂O in the channels (partial disorder).

Alberti A. et al. (1996) [1]

Al_{5.70}Ca_{1.32}H_{32.08}KMgO_{52.04}Si_{12.30}

a = 1.3331, *c* = 0.7593 nm, *c/a* = 0.570, *V* = 1.1686 nm³, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>o</i>	1	0.00903	0.31807	0.3213		non-colinear Si ₂
M2	12 <i>o</i>	1	0.10063	0.43327	0.2089		
O3	6 <i>n</i>	. <i>m</i> .	0.23723	0.76277	0.2558		non-colinear Si ₂
O4	6 <i>n</i>	. <i>m</i> .	0.45953	0.54047	0.2602		non-colinear Si ₂
(OH ₂)5	6 <i>n</i>	. <i>m</i> .	0.77023	0.22977	0.1881		single atom Ca
M6	6 <i>m</i>	<i>m</i> ..	0.00203	0.24307	¹ / ₂		tetrahedron O ₄
O7	6 <i>l</i>	<i>m</i> ..	0.07183	0.39487	0		
(OH ₂)8	6 <i>l</i>	<i>m</i> ..	0.10233	0.43567	0	0.17	
(OH ₂)9	6 <i>l</i>	<i>m</i> ..	0.16633	0.02627	0	0.48	non-colinear (OH ₂) ₂
O10	3 <i>k</i>	<i>mm</i> 2	0.10473	0.89527	¹ / ₂		non-colinear Si ₂
(OH ₂)11	3 <i>k</i>	<i>mm</i> 2	0.56983	0.43017	¹ / ₂		non-colinear Ca ₂
O12	3 <i>k</i>	<i>mm</i> 2	0.87633	0.12367	¹ / ₂		non-colinear Si ₂
(OH ₂)13	3 <i>j</i>	<i>mm</i> 2	0.08873	0.91127	0	0.38	non-colinear (OH ₂) ₂
Ca14	2 <i>i</i>	3 <i>m</i> .	² / ₃	¹ / ₃	0.2812	0.34	
Ca15	2 <i>i</i>	3 <i>m</i> .	² / ₃	¹ / ₃	0.3947	0.32	
(OH ₂)16	2 <i>g</i>	3 <i>m</i> .	0	0	0.2676		single atom Mg
K17	1 <i>d</i>	-6 <i>m</i> 2	¹ / ₃	² / ₃	¹ / ₂		trigonal prism O ₆
Mg18	1 <i>a</i>	-6 <i>m</i> 2	0	0	0		

M2 = 0.71Si + 0.29Al; M6 = 0.63Si + 0.37Al

Transformation from published data: -*x*, -*y*, -*z*; origin shift ²/₃ ¹/₃ 0

Experimental: single crystal, diffractometer, X-rays, wR = 0.046

Remarks: Natural specimen from Poia Creek, Italy. Composition (Na_{0.01}K_{1.09}Mg_{1.11}Ca_{1.07}Sr_{0.01}Ba_{0.01})_—(Al_{5.52}Si_{12.49})O₃₆·17.63H₂O from electron microprobe analysis. 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] Alberti A., Cruciani G., Galli E., Vezzalini G. (1996), Zeolites 17, 457-461.