

KCa<sub>1.5</sub>Mg<sub>0.7</sub>(Al<sub>0.30</sub>Si<sub>0.70</sub>)<sub>18</sub>O<sub>36</sub>[H<sub>2</sub>O]<sub>16.7</sub> *hP*83 (187) *P*-6*m*2 – o<sup>2</sup>n<sup>3</sup>ml<sup>2</sup>k<sup>3</sup>j<sup>2</sup>i<sup>2</sup>gda

**K<sub>0.79</sub>Ca<sub>1.50</sub>Mg<sub>0.70</sub>Al<sub>5.49</sub>Si<sub>12.54</sub>O<sub>36</sub>·16.72H<sub>2</sub>O** [1], offretite, zeolite OFF hydrated

Structural features: (Si,Al)O<sub>4</sub> 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 H<sub>2</sub>O in the channels (partial disorder).

Gualtieri A. et al. (1998) [1]

Al<sub>5.40</sub>Ca<sub>1.52</sub>H<sub>31</sub>K<sub>0.96</sub>Mg<sub>0.97</sub>O<sub>51.50</sub>Si<sub>12.60</sub>

*a* = 1.339, *c* = 0.7598 nm, *c/a* = 0.567, *V* = 1.1798 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>o</i>	1	0.00993	0.31727	0.316		non-colinear Si <sub>2</sub>
M2	12 <i>o</i>	1	0.09983	0.43457	0.2087		tetrahedron O <sub>4</sub>
O3	6 <i>n</i>	. <i>m</i> .	0.23703	0.76287	0.25		non-colinear Si <sub>2</sub>
O4	6 <i>n</i>	. <i>m</i> .	0.45983	0.54007	0.2926		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )5	6 <i>n</i>	. <i>m</i> .	0.76583	0.23417	0.1682		4-vertex polyhedron Ca(OH <sub>2</sub> ) <sub>3</sub>
M6	6 <i>m</i>	<i>m</i> ..	0.24493	0.00137	1/2		tetrahedron O <sub>4</sub>
O7	6 <i>l</i>	<i>m</i> ..	0.07413	0.40227	0		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )8	6 <i>l</i>	<i>m</i> ..	0.19833	0.04207	0	0.26	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O9	3 <i>k</i>	<i>mm</i> 2	0.10013	0.89977	1/2		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )10	3 <i>k</i>	<i>mm</i> 2	0.56703	0.43297	1/2	0.85	non-colinear Ca <sub>2</sub>
O11	3 <i>k</i>	<i>mm</i> 2	0.87303	0.12687	1/2		non-colinear Si <sub>2</sub>
(OH <sub>2</sub> )12	3 <i>j</i>	<i>mm</i> 2	0.09013	0.90987	0	0.81	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
(OH <sub>2</sub> )13	3 <i>j</i>	<i>mm</i> 2	0.58723	0.41277	0	0.32	non-coplanar square (OH <sub>2</sub> ) <sub>4</sub>
Ca14	2 <i>i</i>	3 <i>m</i> .	2/3	1/3	0.2664	0.36	
Ca15	2 <i>i</i>	3 <i>m</i> .	2/3	1/3	0.4021	0.4	
(OH <sub>2</sub> )16	2 <i>g</i>	3 <i>m</i> .	0	0	0.2335		single atom Mg
K17	1 <i>d</i>	-6 <i>m</i> 2	1/3	2/3	1/2	0.96	trigonal prism O <sub>6</sub>
Mg18	1 <i>a</i>	-6 <i>m</i> 2	0	0	0	0.97	colinear (OH <sub>2</sub> ) <sub>2</sub>

M2 = 0.70Si + 0.30Al; M6 = 0.70Si + 0.30Al

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

Experimental: powder, diffractometer, neutrons, wR<sub>p</sub> = 0.014

Remarks: Natural specimen from Fitta, Italy. Composition K<sub>0.79</sub>Mg<sub>0.70</sub>Ca<sub>1.50</sub>(Al<sub>5.49</sub>Si<sub>12.54</sub>O<sub>36</sub>)·16.72H<sub>2</sub>O 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] Gualtieri A., Artioli G., Passaglia E., Bigi S., Viani A., Hanson J.C. (1998), Am. Mineral. 83, 590-606.