

$\text{KCa}_{1.2}\text{Mg}(\text{Al}_{0.30}\text{Si}_{0.70})_{18}\text{O}_{36}[\text{H}_2\text{O}]_{16.6}$	<i>hP80</i>	(187) <i>P-6m2</i> – $\text{o}^2\text{n}^3\text{ml}^2\text{k}^3\text{j}^2\text{gda}$
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$\text{K}_{0.91}\text{Ca}_{1.13}\text{Mg}_{1.02}\text{Al}_{5.41}\text{Si}_{12.62}\text{O}_{36}\cdot 16.64\text{H}_2\text{O}$ [1], offretite, zeolite OFF hydrated
 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]; K at the centers of cancrinite-type cages, hydrated Mg at the centers of gmelinite-type cages, Ca and additional H_2O in the channels (partial disorder). See Fig. IV.15.

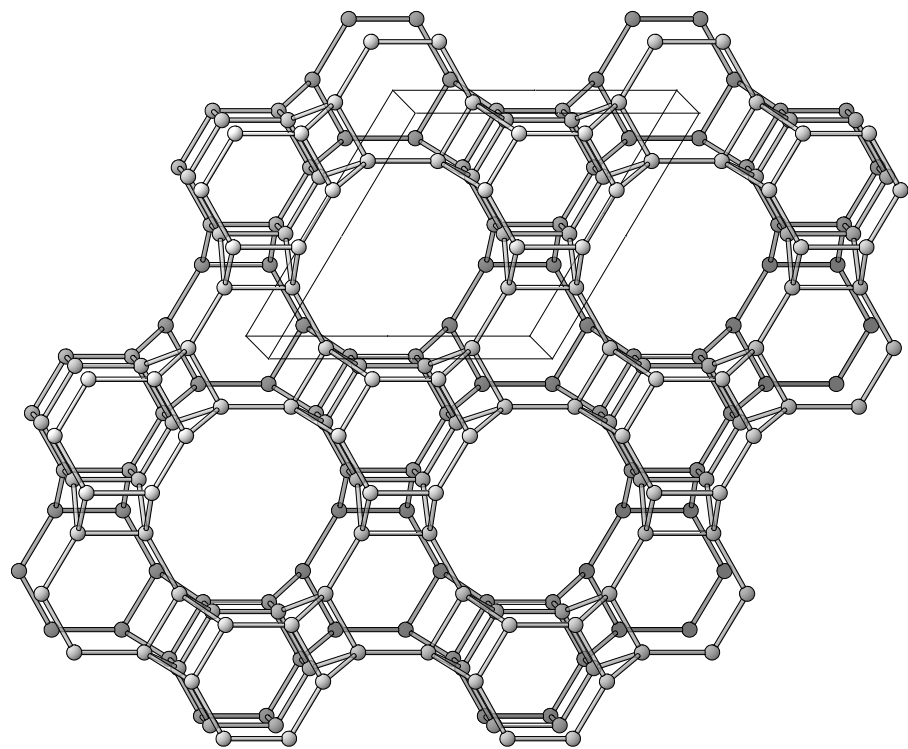


Fig. IV.15. **$\text{K}_{0.91}\text{Ca}_{1.13}\text{Mg}_{1.02}\text{Al}_{5.41}\text{Si}_{12.62}\text{O}_{36}\cdot 16.64\text{H}_2\text{O}$**

OFF-type (Si,Al) framework.

Gualtieri A. et al. (1998) [1]
 $\text{Al}_{5.40}\text{Ca}_{1.50}\text{H}_{32.14}\text{K}_{0.89}\text{Mg}_{0.86}\text{O}_{52.07}\text{Si}_{12.60}$
 $a = 1.3308$, $c = 0.7597$ nm, $c/a = 0.571$, $V = 1.1652$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>o</i>	1	0.00623	0.31877	0.3173		non-colinear Si ₂
M2	12 <i>o</i>	1	0.10223	0.43497	0.2048		tetrahedron O ₄
O3	6 <i>n</i>	. <i>m</i> .	0.23763	0.76237	0.2686		non-colinear Si ₂
O4	6 <i>n</i>	. <i>m</i> .	0.45723	0.54277	0.29		non-colinear Si ₂
(OH ₂)5	6 <i>n</i>	. <i>m</i> .	0.76963	0.23037	0.1603		non-colinear (OH ₂)Ca
M6	6 <i>m</i>	. <i>m</i> ..	0.00273	0.24397	1/2		tetrahedron O ₄
O7	6 <i>l</i>	. <i>m</i> ..	0.06613	0.39757	0		non-colinear Si ₂
(OH ₂)8	6 <i>l</i>	. <i>m</i> ..	0.22043	0.01397	0	0.55	single atom (OH ₂)
O9	3 <i>k</i>	<i>mm</i> 2	0.10463	0.89537	1/2		non-colinear Si ₂

(OH ₂)10	3k	mm2	0.57693	0.42307	$\frac{1}{2}$	0.94	non-colinear Ca ₂
O11	3k	mm2	0.87633	0.12367	$\frac{1}{2}$		non-colinear Si ₂
(OH ₂)12	3j	mm2	0.09093	0.90907	0	0.65	non-colinear (OH ₂) ₂
Ca13	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.2438	0.32	
Ca14	2i	3m.	$\frac{2}{3}$	$\frac{1}{3}$	0.3876	0.43	
(OH ₂)15	2g	3m.	0	0	0.2335		single atom Mg
K16	1d	-6m2	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$	0.89	trigonal prism O ₆
Mg17	1a	-6m2	0	0	0	0.86	trigonal bipyramid (OH ₂) ₅

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

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

Experimental: powder, diffractometer, neutrons, wR_p = 0.025

Remarks: Natural specimen from Fitta, Italy. Composition K_{0.91}Mg_{1.02}Ca_{1.13}(Al_{5.41}Si_{12.62}O₃₆)·16.64H₂O from electron microprobe analysis. We assigned an approximate value to the Al/Si ratio of sites M based on the chemical 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.