| $KCaMg_{1.1}(Al_{0.29}Si_{0.71})_{18}O_{36}[H_2O]_{16.85}$ | *hP*86 | (187) *P*-6*m*2 – $o^2n^4ml^2k^3ji^2gda$ |
|---|---|---|

**$K_{0.88}Ca_{0.97}Mg_{1.06}Al_{5.26}Si_{12.81}O_{36}\cdot 16.85H_2O$** [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).

Gualtieri A. et al. (1998) [1]
$Al_{5.24}Ca_{1.40}H_{27.04}KMgO_{49.52}Si_{12.76}$
$a$ = 1.3293, $c$ = 0.7608 nm, $c/a$ = 0.572, $V$ = 1.1643 $nm^3$, $Z$ = 1

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| O1 | 12*o* | 1 | 0.01243 | 0.31907 | 0.3188 | | non-colinear $Si_2$ |
| M2 | 12*o* | 1 | 0.10213 | 0.43587 | 0.2067 | | tetrahedron $O_4$ |
| O3 | 6*n* | .*m*. | 0.23893 | 0.76087 | 0.234 | | non-colinear $Si_2$ |
| O4 | 6*n* | .*m*. | 0.44843 | 0.55157 | 0.2807 | | non-colinear $Si_2$ |
| $(OH_2)5$ | 6*n* | .*m*. | 0.76903 | 0.23097 | 0.1713 | 0.35 | single atom $(OH_2)$ |
| $(OH_2)6$ | 6*n* | .*m*. | 0.81533 | 0.18467 | 0.1231 | 0.37 | single atom $(OH_2)$ |
| M7 | 6*m* | *m*.. | 0.00423 | 0.24567 | $^1/_2$ | | tetrahedron $O_4$ |
| $(OH_2)8$ | 6*l* | *m*.. | 0.01163 | 0.17097 | 0 | 0.3 | single atom $(OH_2)$ |
| O9 | 6*l* | *m*.. | 0.07043 | 0.39447 | 0 | | non-colinear $Si_2$ |
| O10 | 3*k* | *mm*2 | 0.10623 | 0.89377 | $^1/_2$ | | non-colinear $Si_2$ |
| $(OH_2)11$ | 3*k* | *mm*2 | 0.57543 | 0.42457 | $^1/_2$ | | non-colinear $Ca_2$ |
| O12 | 3*k* | *mm*2 | 0.87883 | 0.12117 | $^1/_2$ | | non-colinear $Si_2$ |
| $(OH_2)13$ | 3*j* | *mm*2 | 0.08963 | 0.91037 | 0 | 0.8 | non-colinear $(OH_2)_2$ |
| Ca14 | 2*i* | 3*m*. | $^2/_3$ | $^1/_3$ | 0.245 | 0.27 | |
| Ca15 | 2*i* | 3*m*. | $^2/_3$ | $^1/_3$ | 0.353 | 0.43 | |
| $(OH_2)16$ | 2*g* | 3*m*. | 0 | 0 | 0.2587 | | single atom Mg |
| K17 | 1*d* | -6*m*2 | $^1/_3$ | $^2/_3$ | $^1/_2$ | | hexagonal prism $O_{12}$ |
| Mg18 | 1*a* | -6*m*2 | 0 | 0 | 0 | | trigonal bipyramid $(OH_2)_5$ |

M2 = 0.709Si + 0.291Al; M7 = 0.709Si + 0.291Al
Transformation from published data: -*x*,-*y*,-*z*; origin shift $^2/_3$ $^1/_3$ 0
Experimental: powder, diffractometer, neutrons, $wR_p$ = 0.018

Remarks: Natural specimen from Mt. Semiol, France. Composition $K_{0.88}Mg_{1.06}Ca_{0.97}(Al_{5.26}Si_{12.81}O_{36})\_\cdot 16.85H_2O$ 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.