| $Ca_2Al(Al_{0.33}Si_{0.67})_3O_3[OH]_{12}[H_2O]_{1.5}$ | *hP*52 | (176) $P6_3/m$ – $i^2hf^3edba$ |
|---|---|---|

**$Ca_4Al_4Si_4O_6(OH)_{24}\cdot 3H_2O$** [1], vertumnite
Structural features: Double slabs of vertex-linked (Si,Al)[O(OH,O)$_3$] tetrahedra with 6-rings alternate with slabs of edge-linked Ca(OH)$_6$ (Ca displaced from the octahedron center and coordinated by an additional OH) and Al(OH)$_6$ octahedra; $H_2O$ between 6-rings in the former slabs.

Galli E., Passaglia E. (1978) [1]
$Al_{2.13}Ca_2H_{14.68}O_{15.72}Si_{1.43}$
$a$ = 0.5755, $c$ = 2.512 nm, $c/a$ = 4.365, $V$ = 0.7205 nm$^3$, $Z$ = 2

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| (OH)1 | 12*i* | 1 | 0.3054 | 0.0554 | 0.0407 | | single atom Al |
| M2 | 12*i* | 1 | 0.335 | 0.2118 | 0.1608 | 0.96 | non-colinear $Si_2$ |
| $(OH_2)$3 | 6*h* | *m*.. | 0.231 | 0.571 | $^1/_4$ | 0.15 | |
| Ca4 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.0212 | | 7-vertex polyhedron $(OH)_7$ |
| M5 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.1208 | | single atom Ca |
| M6 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.6855 | 0.65 | tetrahedron $O(OH)_3$ |
| M7 | 4*e* | 3.. | 0 | 0 | 0.1857 | 0.63 | tetrahedron $O(OH)_3$ |
| O8 | 2*d* | -6.. | $^2/_3$ | $^1/_3$ | $^1/_4$ | 0.73 | colinear $Si_2$ |
| Al9 | 2*b* | -3.. | 0 | 0 | 0 | | octahedron $(OH)_6$ |
| O10 | 2*a* | -6.. | 0 | 0 | $^1/_4$ | 0.78 | colinear $Si_2$ |

M2 = 0.83OH + 0.17O; M5 = 0.5OH + 0.5OH$_2$; M6 = 0.56Si + 0.44Al; M7 = 0.56Si + 0.44Al
Transformation from published data: *y*,*x*,-*z*
Experimental: single crystal, diffractometer, X-rays, R = 0.046

Remarks: Natural specimen from Campomorto, Montalto di Castro, Viterbo, Italy. Refinement using scattering factors corresponding to 0.56Si + 0.435Al + 0.005P for sites M6 and M7, 0.94Ca + 0.0325Al + 0.015Sr + 0.005K + 0.005Na + 0.0025Ba for site Ca4. We assigned an approximate value to the O/OH ratio of site M2 based on the nominal composition. A metrically monoclinic cell with $a$ = 0.5744(5), $b$ = 0.5766(5), $c$ = 2.512(1) nm, $\gamma$ = 119.72(5)° was found; space group (11) $P112_1/m$ was tested and rejected (all atom coordinates within the standard uncertainty). 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] Galli E., Passaglia E. (1978), TMPM, Tschermaks Mineral. Petrogr. Mitt. 25, 33-46.