

$\text{Ba}_4\text{Ca}_{5.4}(\text{Al}_{0.4}\text{Si}_{0.6})_{20}[\text{SO}_4]_3\text{O}_{39}[\text{OH}]_2[\text{H}_2\text{O}]_{0.5}$	<i>hP</i> 110	(189) <i>P</i> -62 <i>m</i> – $1^4k^2j^4h^2gf^2ea$
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Ba₄Ca_{5.4}Al₈Si₁₂O₃₉(SO₄)₃(OH)₂·0.5H₂O [1], wenkite, zeolite WEN

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a WEN-type zeolite framework with cancrinite-type cages (six 4-rings, two planar and three non-planar 6-rings) interconnected via hexagonal prisms, and channels delimited by 10-rings perpendicular to [001] and by 8-rings parallel to [001]; SO₄ tetrahedra, Ca and Ba atoms in the channels.

Wenk H.R. (1973) [1]

$\text{Al}_8\text{Ba}_{3.96}\text{Ca}_{4.92}\text{H}_{2.48}\text{O}_{53.24}\text{S}_3\text{Si}_{12}$

$a = 1.3515$, $c = 0.7465$ nm, $c/a = 0.552$, $V = 1.1808$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>l</i>	1	0.101	0.594	0.106	0.5	non-coplanar triangle O ₂ S
M2	12 <i>l</i>	1	0.1333	0.2668	0.218		tetrahedron O ₄
O3	12 <i>l</i>	1	0.179	0.394	0.318		non-colinear Si ₂
Ca4	12 <i>l</i>	1	0.2243	0.4996	0.012	0.41	
M5	6 <i>k</i>	<i>m</i> ..	0.1378	0.4384	$\frac{1}{2}$		tetrahedron O ₄
O6	6 <i>k</i>	<i>m</i> ..	0.207	0.583	$\frac{1}{2}$		non-coplanar triangle Si ₃
O7	6 <i>j</i>	<i>m</i> ..	0.15	0.294	0		non-colinear Si ₂
O8	6 <i>i</i>	.. <i>m</i>	0.171	0	0.281		non-colinear Si ₂
O9	6 <i>i</i>	.. <i>m</i>	0.57	0	0.173	0.5	non-coplanar triangle O ₂ S
Ba10	6 <i>i</i>	.. <i>m</i>	0.6073	0	0.4788	0.5	
O11	6 <i>i</i>	.. <i>m</i>	0.784	0	0.292		non-colinear Si ₂
(OH)12	4 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.18	0.5	single atom Si
M13	4 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.397	0.5	trigonal bipyramid Si(OH)O ₃
O14	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.4	0	$\frac{1}{2}$		non-colinear Si ₂
O15	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.408	0	0		single atom S
S16	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.5169	0	0		7-vertex polyhedron O ₇
Ba17	2 <i>e</i>	3.. <i>m</i>	0	0	0.485	0.48	
(OH ₂)18	1 <i>a</i>	-62 <i>m</i>	0	0	0	0.24	trigonal prism O ₆

M2 = 0.6Si + 0.4Al; M5 = 0.6Si + 0.4Al; M13 = 0.6Si + 0.4Al

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

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

Remarks: Natural specimen from Ivrea region, the Alps. Cation content Ba_{3.96}(Ca_{4.89}Na_{0.68}K_{0.14})Al_{8.64}Si_{11.36}S_{2.61} from electron microprobe analysis (of another sample). Cell parameters from [2]. Average structure; the authors state that true symmetry is trigonal, space group (157) *P*31*m*. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 of [1] the occupancy of former O(10) is misprinted as $\frac{1}{2}$ instead of 1 (from the description of the structure).

References: [1] Wenk H.R. (1973), *Z. Kristallogr.* 137, 113-126. [2] Wenk H.R. (1966), *Schweiz. Mineral. Petrogr. Mitt.* 46, 85-88.