$(K_{0.125}Ba_{0.875})_4(Na_{0.083}Ca_{0.917})_6(Al_{0.44}Si_{0.55})_{20}[SO_4]_3O_{41}[OH]_2[H_2O]$ *hP*126 (189) *P*-62*m* – $l^6k^2j^2i^2h^2gf^2a$

$(Ba,K)_4(Ca,Na)_6(Si,Al)_{20}O_{41}(SO_4)_3(OH)_2 \cdot H_2O$ [1], wenkite, zeolite WEN
Structural features: $(Si,Al)O_4$ 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]; SO_4 tetrahedra and (Ba,K) and (Ca,Na) atoms in the channels.

Merlino S. (1974) [1]
$Al_9Ba_{3.50}Ca_{5.50}H_2K_{0.50}Na_{0.50}O_{55}S_3Si_{11}$
a = 1.3511, c = 0.7462 nm, c/a = 0.552, V = 1.1797 nm^3, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*l*	1	0.019	0.421	0.451	0.25	
O2	12*l*	1	0.092	0.591	0.346	0.25	
O3	12*l*	1	0.114	0.606	0.426	0.25	
M4	12*l*	1	0.133	0.2666	0.2822		tetrahedron O_4
O5	12*l*	1	0.177	0.392	0.183		non-colinear Si_2
O6	12*l*	1	0.401	0.447	0.342	0.25	
O7	6*k*	*m*..	0.151	0.296	$^1/_2$		non-colinear Si_2
M8	6*k*	*m*..	0.2245	0.4988	$^1/_2$		
M9	6*j*	*m*..	0.1372	0.438	0		tetrahedron O_4
O10	6*j*	*m*..	0.202	0.58	0		non-coplanar triangle Si_3
O11	6*i*	..*m*	0.17	0	0.225		non-colinear Si_2
O12	6*i*	..*m*	0.784	0	0.206		non-colinear Si_2
M13	4*h*	3..	$^1/_3$	$^2/_3$	0.103	0.5	trigonal bipyramid SiO_4
M14	4*h*	3..	$^1/_3$	$^2/_3$	0.33		single atom Si
S15	3*g*	*m*2*m*	0.52	0	$^1/_2$		
O16	3*f*	*m*2*m*	0.399	0	0		non-colinear Si_2
M17	3*f*	*m*2*m*	0.6068	0	0		
M18	1*a*	-62*m*	0	0	0		trigonal prism O_6

M4 = 0.55Si + 0.45Al; M8 = 0.917Ca + 0.083Na; M9 = 0.55Si + 0.45Al; M13 = 0.55Si + 0.45Al; M14 = 0.5O + 0.5OH; M17 = 0.875Ba + 0.125K; M18 = 0.875Ba + 0.125K
Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.098

Remarks: Natural specimen from Candoglia, Italy. H_2O not located. Cell parameters from [2]. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Average structure; the author states that true symmetry is probably lower due to ordering Si/Al. Space groups (150) *P*321 and (157) *P*31*m* were tested and rejected.

References: [1] Merlino S. (1974), Acta Crystallogr. B 30, 1262-1266. [2] Wenk H.R. (1966), Schweiz. Mineral. Petrogr. Mitt. 46, 85-88.