$Na_{20}Ca_9(Al_{0.5}Si_{0.5})_{48}O_{96}[SO_4]_{5.3}[CO_3]_{0.7}Cl_2[H_2O]_4$	*hP*250	(186) $P6_3mc$ – $d^8c^{22}b^7a^4$

$K_{0.2}Na_{4.5}Ca_{2.5}Al_6Si_6O_{23.6}(CO_3)_{0.2}(SO_4)_{1.4}Cl_{1.4}\cdot 2.6H_2O$ [1], afghanite, zeolite AFG
Structural features: $(Al,Si)O_4$ tetrahedra share vertices to form an AFG-type zeolite framework (6-rings in ACACBCBC stacking) with cancrinite- (six 4-rings, two planar and three non-planar 6-rings) and liottite-type cages (two 4-rings and seventeen 6-rings); Cl at the centers of cancrinite cages, SO_4 tetrahedra and CO_3 trigonal units (partial disorder) in large cages.

Pobedimskaya E.A. et al. (1991) [1]
$Al_{24}C_{0.67}Ca_{9.80}Cl_2H_8Na_{22.02}O_{118.02}S_{4.83}Si_{24}$
$a = 1.2761$, $c = 2.1416$ nm, $c/a = 1.678$, $V = 3.0202$ nm^3, $Z = 1$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
M1	12*d*	1	0.0001	0.2572	0.0077		tetrahedron O_4
M2	12*d*	1	0.0061	0.2586	0.2574		tetrahedron O_4
O3	12*d*	1	0.0163	0.3332	0.0756		non-colinear Al_2
M4	12*d*	1	0.0746	0.41	0.3836		tetrahedron O_4
O5	12*d*	1	0.3309	0.0023	0.3268		non-colinear Al_2
O6	12*d*	1	0.3453	0.009	0.2008		non-colinear Al_2
O7	12*d*	1	0.3481	0.0047	0.4487		non-colinear Al_2
M8	12*d*	1	0.4091	0.077	0.1313		tetrahedron O_4
O9	6*c*	.*m*.	0.1132	0.8868	0.0149		non-colinear Al_2
O10	6*c*	.*m*.	0.1184	0.8816	0.2585		non-colinear Al_2
Na11	6*c*	.*m*.	0.2017	0.7983	0.1437	0.33	
O12	6*c*	.*m*.	0.2222	0.7778	0.3917		non-colinear Al_2
Na13	6*c*	.*m*.	0.2238	0.7762	0.1248	0.66	
O14	6*c*	.*m*.	0.281	0.719	0.0404	0.27	non-colinear OS
O15	6*c*	.*m*.	0.397	0.603	0.2084	0.41	single atom S
O16	6*c*	.*m*.	0.4589	0.5411	0.3879		non-colinear Al_2
Na17	6*c*	.*m*.	0.4707	0.5293	0.0112	0.85	
Na18	6*c*	.*m*.	0.4907	0.5093	0.253	0.83	
Ca19	6*c*	.*m*.	0.4949	0.5051	0.0172	0.14	
Ca20	6*c*	.*m*.	0.5162	0.4838	0.2609	0.16	
O21	6*c*	.*m*.	0.551	0.449	0.1417		non-colinear Al_2
O22	6*c*	.*m*.	0.6116	0.3884	0.3255		single atom S
O23	6*c*	.*m*.	0.613	0.387	0.4574	0.33	non-coplanar triangle O_2S
O24	6*c*	.*m*.	0.636	0.364	0.2431	0.33	non-coplanar triangle O_2S
O25	6*c*	.*m*.	0.728	0.272	0.4794	0.33	4-vertex polyhedron O_3S
Na26	6*c*	.*m*.	0.784	0.216	0.3844	0.9	
O27	6*c*	.*m*.	0.788	0.212	0.1347		non-colinear Al_2
Na28	6*c*	.*m*.	0.83	0.17	0.3694	0.1	
O29	6*c*	.*m*.	0.8814	0.1186	0.0061		non-colinear Al_2
O30	6*c*	.*m*.	0.8899	0.1101	0.2659		non-colinear Al_2
M31	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0087		9-vertex polyhedron O_9
S32	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2235	0.75	tetrahedron O_4
O33	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2906		single atom S
Ca34	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.3931		hexagonal bipyramid $O_7(OH_2)$
(OH_2)35	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.512		colinear Ca_2
Ca36	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.6368		10-vertex polyhedron $O_9(OH_2)$
S37	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.7996		trigonal prism O_6
Ca38	2*a*	3*m*.	0	0	0.0		hexagonal bipyramid $(OH_2)O_6Cl$
Cl39	2*a*	3*m*.	0	0	0.1337		colinear Ca_2
Ca40	2*a*	3*m*.	0	0	0.2515		hexagonal bipyramid $O_6Cl(OH_2)$

$(OH_2)41$	2*a*	3*m*.	0	0	0.3828	colinear Ca_2

M1 = 0.50Al + 0.50Si; M2 = 0.50Al + 0.50Si; M4 = 0.50Al + 0.50Si; M8 = 0.50Al + 0.50Si; M31 = 0.667S + 0.333C
Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 0.2406
Experimental: single crystal, diffractometer, X-rays, R = 0.069

Remarks: Natural specimen from the Baykal region, Russia. Composition $Na_{4.5}Ca_{2.5}K_{0.2}Al_6Si_6O_{23.6}$_ $(SO_4)_{1.4}(CO_3)_{0.2}Cl_{1.4}{\cdot}2.6H_2O$ from chemical analysis. The authors state that CO_3 may statistically substitute for SO_4 on site M31, refined value occ(M31) = 0.90 considering f(S). We assigned approximate values to the Al/Si ratio of sites M1, M2, M4, and M8, and to the C/S ratio of site M31, based on the nominal composition. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances for partly occupied site(s). The same data are also reported in [2]. The structure was redetermined in space group (159) *P*31*c* in [3]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Pobedimskaya E.A., Rastsvetaeva R.K., Terent'eva L.E., Sapozhnikov A.N. (1991), Dokl. Akad. Nauk SSSR 320, 882-886. [2] Rastsvetaeva R.K., Pobedimskaya E.A., Terent'eva L.E., Sapozhnikov A.N. (1993), Crystallogr. Rep. 38, 185-189 (Kristallografiya 38(2), 94-103). [3] Ballirano P., Bonaccorsi E., Maras A., Merlino S (1997), Eur. J. Mineral. 9, 21-30.