$Na_7Ca_3[SO_4]_6[OH][H_2O]_{0.8}$	*hP*43	(174) *P*-6 – $l^2k^4j^4ihga$

$Na_7Ca_3(SO_4)_6(OH)(H_2O)_{0.8}$ [1], cesanite, apatite family
Structural features: Infinite columns of base-linked distorted NaO_6 and $(Na,Ca)O_6$ trigonal prisms share atoms with SO_4 tetrahedra to form a 3D-framework; (OH,OH_2) in infinite columns of face-linked $(Ca,Na)_6$ and $(Na,Ca)_6$ octahedra parallel to [001] (partial disorder, O close to trigonal coordination).

Piotrowski A. et al. (2002) [1]
$Ca_{2.98}H_{2.53}Na_{7.02}O_{25.76}S_6$
$a = 0.9463$, $c = 0.69088$ nm, $c/a = 0.73$, $V = 0.5358$ nm^3, $Z = 1$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	6*l*	1	0.0703	0.329	0.172		single atom S
O2	6*l*	1	0.335	0.2573	0.3302		single atom S
M3	3*k*	*m*..	0.0087	0.2515	$^1/_2$		
O4	3*k*	*m*..	0.3193	0.4709	$^1/_2$		single atom S
S5	3*k*	*m*..	0.3903	0.3643	$^1/_2$		tetrahedron O_4
O6	3*k*	*m*..	0.5408	0.1119	$^1/_2$		single atom S
S7	3*j*	*m*..	0.0264	0.3909	0		tetrahedron O_4
O8	3*j*	*m*..	0.1072	0.5678	0		single atom S
M9	3*j*	*m*..	0.2644	0.2512	0		pentagonal bipyramid $O_6(OH)$
O10	3*j*	*m*..	0.4732	0.1525	0		single atom S
M11	2*i*	3..	$^2/_3$	$^1/_3$	0.2461		octahedron O_6
Na12	2*h*	3..	$^1/_3$	$^2/_3$	0.2537		octahedron O_6
M13	2*g*	3..	0	0	0.4579	0.585	
M14	1*a*	-6..	0	0	0	0.59	coplanar triangle Ca_3

M3 = 0.83Na + 0.17Ca; M9 = 0.71Ca + 0.29Na; M11 = 0.83Na + 0.17Ca; M13 = 0.56OH + 0.44OH_2; M14 = 0.56OH + 0.44OH_2
Transformation from published data: *y*,*x*,*z*
Experimental: single crystal, diffractometer, X-rays, R = 0.047

Remarks: Natural specimen from Cesano area, Latium, Italy. We assigned an approximate value to the OH/OH_2 ratio of sites M13 and M14 based on the nominal composition. Space group (176) $P6_3/m$, used in [2], was tested and rejected both for natural and synthetic cesanite. 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] Piotrowski A., Kahlenberg V., Fischer R.X., Lee Y., Parise J.B. (2002), Am. Mineral. 87, 715-720. [2] Tazzoli V. (1983), Mineral. Mag. 47, 59-63.