



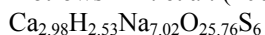
hP43

(174) $P-6 - I^2k^4j^4ihga$

Na₇Ca₃(SO₄)₆(OH)(H₂O)_{0.8} [1], cesanite, apatite family

Structural features: Infinite columns of base-linked distorted NaO₆ and (Na,Ca)O₆ trigonal prisms share atoms with SO₄ tetrahedra to form a 3D-framework; (OH,OH₂) 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]



$a = 0.9463$, $c = 0.69088$ nm, $c/a = 0.73$, $V = 0.5358$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>l</i>	1	0.0703	0.329	0.172		single atom S
O2	6 <i>l</i>	1	0.335	0.2573	0.3302		single atom S
M3	3 <i>k</i>	<i>m</i> ..	0.0087	0.2515	¹ / ₂		
O4	3 <i>k</i>	<i>m</i> ..	0.3193	0.4709	¹ / ₂		single atom S
S5	3 <i>k</i>	<i>m</i> ..	0.3903	0.3643	¹ / ₂		tetrahedron O ₄
O6	3 <i>k</i>	<i>m</i> ..	0.5408	0.1119	¹ / ₂		single atom S
S7	3 <i>j</i>	<i>m</i> ..	0.0264	0.3909	0		tetrahedron O ₄
O8	3 <i>j</i>	<i>m</i> ..	0.1072	0.5678	0		single atom S
M9	3 <i>j</i>	<i>m</i> ..	0.2644	0.2512	0		pentagonal bipyramid O ₆ (OH)
O10	3 <i>j</i>	<i>m</i> ..	0.4732	0.1525	0		single atom S
M11	2 <i>i</i>	3..	² / ₃	¹ / ₃	0.2461		octahedron O ₆
Na12	2 <i>h</i>	3..	¹ / ₃	² / ₃	0.2537		octahedron O ₆
M13	2 <i>g</i>	3..	0	0	0.4579	0.585	
M14	1 <i>a</i>	-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 + 0.44OH₂; M14 = 0.56OH + 0.44OH₂

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/OH₂ 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.