

$\text{Na}_{3.2}\text{Ca}_{1.8}[\text{SO}_4]_3\text{Cl}_{0.8}$ 

hP50

(176)  $P6_3/m - ih^4fe^2b$  $\text{Na}_{6.39}\text{Ca}_{3.61}(\text{SO}_4)_6\text{Cl}_{1.61}$  [1], apatite family

Structural features: Infinite columns of base-linked (Na,Ca) $\text{O}_6\text{O}_3$  tricapped trigonal prisms share atoms with  $\text{SO}_4$  tetrahedra to form a 3D-framework; Cl in infinite columns of face-linked (Ca,Na) $_6$  octahedra parallel to [001] (partial disorder).

Piotrowski A. et al. (2002) [1]

 $\text{Ca}_{1.81}\text{Cl}_{0.80}\text{Na}_{3.19}\text{O}_{12}\text{S}_3$  $a = 0.95423$ ,  $c = 0.68429$  nm,  $c/a = 0.717$ ,  $V = 0.5396$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.3493	0.083	0.0776		single atom S
O2	6h	m..	0.1472	0.4759	$\frac{1}{4}$		single atom S
M3	6h	m..	0.2474	0.2578	$\frac{1}{4}$		
S4	6h	m..	0.3997	0.0294	$\frac{1}{4}$		tetrahedron O <sub>4</sub>
O5	6h	m..	0.5757	0.1103	$\frac{1}{4}$		single atom S
M6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.003		trigonal prism O <sub>6</sub>
Cl7	4e	3..	0	0	0.088	0.147	
Cl8	4e	3..	0	0	0.1695	0.135	
Cl9	2b	-3..	0	0	0	0.24	

 $M3 = 0.512\text{Ca} + 0.488\text{Na}$ ;  $M6 = 0.864\text{Na} + 0.136\text{Ca}$ Transformation from published data:  $y, x, -z$ 

Experimental: single crystal, diffractometer, X-rays, R = 0.055

Remarks: A similar structure is proposed for human tooth enamel in [2], where, however,  $\text{CO}_3$  could not be located. Short interatomic distances for partly occupied site(s).

References: [1] Piotrowski A., Kahlenberg V., Fischer R.X. (2002), J. Solid State Chem. 163, 398-405.  
[2] Young R.A., Mackie P.E. (1980), Mater. Res. Bull. 15, 17-29.