

$(\text{Na}_{0.65}\text{Ca}_{0.35})_5[\text{SO}_4]_3\text{Cl}_{0.29}\text{F}_{0.45}$ *hP48* $(176) P6_3/m - \text{ih}^4\text{feba}$ $\text{Na}_{6.52}\text{Ca}_{3.48}(\text{SO}_4)_6\text{Cl}_{0.58}\text{F}_{0.90}$ [1], apatite family

Structural features: Infinite columns of base-linked NaO_6O_3 tricapped trigonal prisms (partial substitution Ca/Na ignored) share atoms with SO_4 tetrahedra to form a 3D-framework; F (in trigonal coordination) and Cl (at and displaced from octahedron centers) in infinite columns of face-linked $(\text{Ca},\text{Na})_6$ octahedra parallel to [001] (partial disorder).

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

 $\text{Ca}_{1.74}\text{Cl}_{0.29}\text{F}_{0.45}\text{Na}_{3.26}\text{O}_{12}\text{S}_3$ $a = 0.94859$, $c = 0.68837$ nm, $c/a = 0.726$, $V = 0.5364$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.3411	0.0808	0.0793		single atom S
O2	6 <i>h</i>	<i>m</i> ..	0.1511	0.4708	$\frac{1}{4}$		single atom S
M3	6 <i>h</i>	<i>m</i> ..	0.2428	0.2533	$\frac{1}{4}$		
S4	6 <i>h</i>	<i>m</i> ..	0.3942	0.027	$\frac{1}{4}$		tetrahedron O ₄
O5	6 <i>h</i>	<i>m</i> ..	0.5714	0.1066	$\frac{1}{4}$		single atom S
M6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0055		trigonal prism O ₆
Cl7	4 <i>e</i>	3..	0	0	0.138	0.102	
Cl8	2 <i>b</i>	-3..	0	0	0	0.09	
F9	2 <i>a</i>	-6..	0	0	$\frac{1}{4}$	0.45	

 $\text{M3} = 0.564\text{Ca} + 0.436\text{Na}$; $\text{M6} = 0.975\text{Na} + 0.025\text{Ca}$ Transformation from published data: *y*,*x*,*-z*Experimental: single crystal, diffractometer, X-rays, $R = 0.057$

Remarks: 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.