

$\text{Sr}_{2.5}\text{Ca}_{2.5}[\text{PO}_4]_3\text{Cl}$ $hP52$ $(176) P6_3/m - ih^5f^2b$ **(Ca,Sr)₅(PO₄)₃Cl** [1], apatite family

Structural features: Infinite columns of base-linked (Ca,Sr)O₆O₃ tricapped trigonal prisms (distinct positions for Ca and Sr) share atoms with PO₄ tetrahedra to form a 3D-framework; infinite columns of face-linked Cl(Sr,Ca)₆ octahedra in channels parallel to [001] (distinct positions for Ca and Sr).

Sudarsanan K., Young R.A. (1980) [1]

 $\text{Ca}_{2.57}\text{Cl}_{0.93}\text{O}_{11.49}\text{P}_{2.92}\text{Sr}_{2.42}$ $a = 0.9737$, $c = 0.7022$ nm, $c/a = 0.721$, $V = 0.5766$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	1	0.3573	0.0852	0.0739	0.933	single atom P
O2	6h	<i>m</i> ..	0.1462	0.4952	¹ / ₄		single atom P
Sr3	6h	<i>m</i> ..	0.2472	0.2595	¹ / ₄	0.678	
Ca4	6h	<i>m</i> ..	0.2561	0.2535	¹ / ₄	0.32	
P5	6h	<i>m</i> ..	0.41	0.0329	¹ / ₄	0.973	tetrahedron O ₄
O6	6h	<i>m</i> ..	0.5917	0.1281	¹ / ₄	0.963	single atom P
Sr7	4f	3..	¹ / ₃	² / ₃	0.0002	0.193	
Ca8	4f	3..	¹ / ₃	² / ₃	0.002	0.806	
Cl9	2b	-3..	0	0	0	0.926	

Transformation from published data: *y*,*x*,*-z*

Experimental: single crystal, diffractometer, X-rays, R = 0.062

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Sudarsanan K., Young R.A. (1980), Acta Crystallogr. B 36, 1525-1530.