

$\text{Sr}_{0.3}\text{Ca}_{4.7}[\text{PO}_4]_3\text{Cl}$ *hP50*(176) $P6_3/m - ih^5fe$ **(Ca,Sr)₅(PO₄)₃Cl** [1], apatite family

Structural features: Infinite columns of base-linked CaO_6O_3 tricapped trigonal prisms share atoms with PO_4 tetrahedra to form a 3D-framework; infinite columns of face-linked $\text{Cl}(\text{Ca,Sr})_6$ octahedra parallel to [001] (split Cl site, distinct positions for Ca and Sr).

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

 $\text{Ca}_{4.40}\text{Cl}_{0.95}\text{O}_{11.71}\text{P}_3\text{Sr}_{0.35}$ $a = 0.9653$, $c = 0.6777$ nm, $c/a = 0.702$, $V = 0.5469$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.3551	0.0866	0.067	0.984	single atom P
O2	6 <i>h</i>	<i>m</i> ..	0.1479	0.4935	$\frac{1}{4}$	0.97	single atom P
Sr3	6 <i>h</i>	<i>m</i> ..	0.245	0.253	$\frac{1}{4}$	0.116	
Ca4	6 <i>h</i>	<i>m</i> ..	0.2605	0.2543	$\frac{1}{4}$	0.826	
P5	6 <i>h</i>	<i>m</i> ..	0.409	0.0327	$\frac{1}{4}$		tetrahedron O ₄
O6	6 <i>h</i>	<i>m</i> ..	0.5937	0.1285	$\frac{1}{4}$	0.965	single atom P
Ca7	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0034	0.96	trigonal prism O ₆
Cl8	4 <i>e</i>	3..	0	0	0.0367	0.474	

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

Experimental: single crystal, diffractometer, X-rays, R = 0.032

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

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