

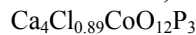
hP46

(176) $P6_3/m - \text{ih}^4\text{fea}$

(Ca,Co)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; Cl in infinite columns of face-linked $(\text{Ca,Co})_6$ octahedra parallel to [001] (partial disorder).

Anderson J.B., Kostiner E. (1987) [1]



$a = 0.9625$, $c = 0.6747$ nm, $c/a = 0.701$, $V = 0.5413$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12i	1	0.3527	0.0865	0.0673		single atom P
O2	6h	<i>m</i> ..	0.1491	0.4921	$\frac{1}{4}$		single atom P
M3	6h	<i>m</i> ..	0.2616	0.2573	$\frac{1}{4}$		octahedron O ₅ Cl
P4	6h	<i>m</i> ..	0.4066	0.0323	$\frac{1}{4}$		tetrahedron O ₄
O5	6h	<i>m</i> ..	0.5916	0.1265	$\frac{1}{4}$		single atom P
Ca6	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0038		trigonal prism O ₆
Cl7	4e	3..	0	0	0.063	0.395	
Cl8	2a	-6..	0	0	$\frac{1}{4}$	0.1	

$M3 = 0.667\text{Ca} + 0.333\text{Co}$

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

Experimental: single crystal, diffractometer, X-rays, R = 0.054

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

References: [1] Anderson J.B., Kostiner E. (1987), J. Solid State Chem. 66, 343-349.