

$\text{Ca}_{10}[\text{PO}_4]_6\text{O}$	<i>hP41</i>	(174) <i>P</i> -6 – $1^2k^4j^4hge$
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$\text{Ca}_{10}(\text{PO}_4)_6\text{O}$ [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; additional O (trigonal coordination) in infinite columns of face-linked Ca_6 octahedra in channels parallel to [001].

Henning P.A. et al. (1999) [1]

$\text{Ca}_{10}\text{O}_{25}\text{P}_6$

$a = 0.9432$, $c = 0.6881$ nm, $c/a = 0.730$, $V = 0.5301$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>l</i>	1	0.01397	0.42183	0.3226		single atom P
O2	6 <i>l</i>	1	0.31797	0.24383	0.1751		single atom P
P3	3 <i>k</i>	<i>m</i> ..	0.06717	0.36323	$\frac{1}{2}$		tetrahedron O ₄
O4	3 <i>k</i>	<i>m</i> ..	0.18347	0.00603	$\frac{1}{2}$		single atom P
O5	3 <i>k</i>	<i>m</i> ..	0.25567	0.45613	$\frac{1}{2}$		single atom P
Ca6	3 <i>k</i>	<i>m</i> ..	0.38307	0.29223	$\frac{1}{2}$		4-vertex polyhedron O ₄
O7	3 <i>j</i>	<i>m</i> ..	0.07787	0.21023	0		single atom P
P8	3 <i>j</i>	<i>m</i> ..	0.26517	0.30443	0		tetrahedron O ₄
O9	3 <i>j</i>	<i>m</i> ..	0.33807	0.48883	0		single atom P
Ca10	3 <i>j</i>	<i>m</i> ..	0.42057	0.07853	0		pentagonal bipyramid O ₇
Ca11	2 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.2487		tricapped trigonal prism O ₉
Ca12	2 <i>g</i>	3..	0	0	0.25162		tricapped trigonal prism O ₉
O13	1 <i>e</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	0		coplanar triangle Ca ₃

Transformation from published data: -*y*, -*x*, -*z*; origin shift $\frac{1}{3}$ $\frac{2}{3}$ $\frac{1}{2}$

Experimental: thin film, electron diffraction

Remarks: Approximate cell parameters from [2], determined on hydroxylapatite.

References: [1] Henning P.A., Landa Canovas A.R., Larsson A.K., Lidin S. (1999), Acta Crystallogr. B 55, 170-176. [2] Kay M.I., Young R.A., Posner A.S. (1964), Nature (London) 204, 1050-1052.