

Ca ₁₅ [PO ₄] ₉ IO	<i>hP</i> 134	(176) <i>P</i> 6 ₃ / <i>m</i> – i ⁷ h ⁴ f ³ e ³ b
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Ca₁₅(PO₄)₉OI [1], apatite family

Structural features: Infinite columns of base-linked CaO₆O₃ tricapped trigonal prisms share atoms with PO₄ tetrahedra to form a 3D-framework; I and additional O in infinite columns of face-linked Ca₆ octahedra parallel to [001] (partial order).

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

Ca₁₅I_{1.05}O_{36.98}P₉

a = 0.9567, *c* = 2.0754 nm, *c/a* = 2.169, *V* = 1.6451 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
P1	12 <i>i</i>	1	0.0309	0.3999	0.0826		tetrahedron O ₄
O2	12 <i>i</i>	1	0.073	0.318	0.1366		single atom P
O3	12 <i>i</i>	1	0.0919	0.375	0.0186		single atom P
O4	12 <i>i</i>	1	0.1249	0.5848	0.093		single atom P
Ca5	12 <i>i</i>	1	0.2765	0.2621	0.0859		pentagonal bipyramid O ₇
O6	12 <i>i</i>	1	0.36	0.268	0.1901		single atom P
O7	12 <i>i</i>	1	0.4886	0.1533	0.083		single atom P
Ca8	6 <i>h</i>	<i>m</i> ..	0.0041	0.2435	¹ / ₄		
O9	6 <i>h</i>	<i>m</i> ..	0.328	0.481	¹ / ₄		single atom P
P10	6 <i>h</i>	<i>m</i> ..	0.4048	0.3731	¹ / ₄		tetrahedron O ₄
O11	6 <i>h</i>	<i>m</i> ..	0.527	0.117	¹ / ₄		single atom P
Ca12	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.0008		tricapped trigonal prism O ₉
Ca13	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.1703		trigonal prism O ₆
Ca14	4 <i>f</i>	3..	¹ / ₃	² / ₃	0.6665		tricapped trigonal prism O ₉
O15	4 <i>e</i>	3..	0	0	0.116	0.14	single atom I
I16	4 <i>e</i>	3..	0	0	0.1716	0.174	colinear O ₂
O17	4 <i>e</i>	3..	0	0	0.237	0.35	
I18	2 <i>b</i>	-3..	0	0	0	0.7	colinear O ₂

Transformation from published data: *y*,*x*,*-z*; origin shift 0 0 ¹/₂

Experimental: single crystal, diffractometer, X-rays, *R* = 0.045, *T* = 293 K

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

References: [1] Henning P.A., Lidin S., Petricek V. (1999), Acta Crystallogr. B 55, 165-169.