

$\text{Pb}_{4.5}[\text{PO}_4]_3$	<i>hP40</i>	(176) $P6_3/m - \text{ih}^4\text{f}$
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Pb₉(PO₄)₆ [1], apatite family

Structural features: Infinite columns of base-linked PbO₆O₃ tricapped trigonal prisms (partial vacancies ignored) share atoms with PO₄ tetrahedra to form a 3D-framework; infinite columns of empty face-linked Pb₆ octahedra in channels parallel to [001]. Alternatively, PO₄ tetrahedra share vertices with :PbO₃ ψ-tetrahedra to form a 3D-framework.

Hata M. et al. (1980) [1]

$\text{O}_{12}\text{P}_3\text{Pb}_{4.50}$

$a = 0.9826$, $c = 0.7357$ nm, $c/a = 0.749$, $V = 0.6152$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.347	0.0805	0.0806		single atom P
O2	6 <i>h</i>	<i>m</i> ..	0.1638	0.4769	$\frac{1}{4}$		single atom P
Pb3	6 <i>h</i>	<i>m</i> ..	0.2518	0.2548	$\frac{1}{4}$		single atom O
P4	6 <i>h</i>	<i>m</i> ..	0.3951	0.0196	$\frac{1}{4}$		tetrahedron O ₄
O5	6 <i>h</i>	<i>m</i> ..	0.5781	0.0969	$\frac{1}{4}$		single atom P
Pb6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0054	0.75	tricapped trigonal prism O ₉

Experimental: single crystal, diffractometer, X-rays, R = 0.043

References: [1] Hata M., Marumo F., Iwai S.I., Aoki H. (1980), Acta Crystallogr. B 36, 2128-2130.