

$\text{Er}_3\text{Pb}_{1.5}[\text{SiO}_4]_3$ *hP40*(176) $P6_3/m - ih^4f$ **Er₆Pb₃(SiO₄)₆** [1], apatite family

Structural features: Infinite columns of base-linked PbO₆O₃ tricapped trigonal prisms (partial vacancies ignored) share atoms with SiO₄ tetrahedra to form a 3D-framework; infinite columns of empty face-linked Er₆ octahedra in channels parallel to [001].

Ansell G.B., Wanklyn B.M. (1976) [1]

 $\text{Er}_3\text{O}_{12}\text{Pb}_{1.50}\text{Si}_3$ $a = 0.9642$, $c = 0.678$ nm, $c/a = 0.703$, $V = 0.5459$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.3703	0.0924	0.0499		single atom Si
O2	6 <i>h</i>	<i>m</i> ..	0.1576	0.5156	$\frac{1}{4}$		single atom Si
Er3	6 <i>h</i>	<i>m</i> ..	0.2486	0.2349	$\frac{1}{4}$		non-coplanar triangle O ₃
Si4	6 <i>h</i>	<i>m</i> ..	0.4175	0.0292	$\frac{1}{4}$		tetrahedron O ₄
O5	6 <i>h</i>	<i>m</i> ..	0.6125	0.1487	$\frac{1}{4}$		single atom Si
Pb6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0044	0.75	tricapped trigonal prism O ₉

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

Experimental: single crystal, diffractometer, X-rays, R = 0.044

Remarks: We assume that in [1] the *y*-coordinate of former O(2) is misprinted as 0.4338 instead of 0.4638 (better interatomic distances).

References: [1] Ansell G.B., Wanklyn B.M. (1976), J. Chem. Soc., Chem. Commun. 1976, 706-707.