

$(\text{Sr}_{0.998}\text{Eu}_{0.002})_5[\text{PO}_4]_3\text{Cl}_{0.5}\text{F}_{0.5}$

*hP48*

(176)  $P6_3/m - ih^4fe^2$

**Sr<sub>4.99</sub>Eu<sub>0.01</sub>(PO<sub>4</sub>)<sub>3</sub>Cl<sub>0.5</sub>F<sub>0.5</sub>** [1], apatite family

Structural features: Infinite columns of base-linked (Sr,Eu)O<sub>6</sub>O<sub>3</sub> tricapped trigonal prisms share atoms with PO<sub>4</sub> tetrahedra to form a 3D-framework; Cl (near octahedron centers) and F (near trigonal voids) in infinite columns of face-linked (Sr,Eu)<sub>6</sub> octahedra parallel to [001] (partial disorder).

Nötzold D., Wulff H. (1998) [1]

Cl<sub>0.50</sub>Eu<sub>0.01</sub>F<sub>0.50</sub>O<sub>12</sub>P<sub>3</sub>Sr<sub>4.99</sub>

$a = 0.98042$ ,  $c = 0.72357$  nm,  $c/a = 0.738$ ,  $V = 0.6023$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.3365	0.0601	0.0693		single atom P
O2	6 <i>h</i>	<i>m</i> ..	0.144	0.4756	<sup>1</sup> / <sub>4</sub>		single atom P
M3	6 <i>h</i>	<i>m</i> ..	0.2484	0.2591	<sup>1</sup> / <sub>4</sub>		
P4	6 <i>h</i>	<i>m</i> ..	0.4002	0.0324	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
O5	6 <i>h</i>	<i>m</i> ..	0.5903	0.1282	<sup>1</sup> / <sub>4</sub>		single atom P
M6	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0002		trigonal prism O <sub>6</sub>
Cl7	4 <i>e</i>	3..	0	0	0.0426	0.25	
F8	4 <i>e</i>	3..	0	0	0.2045	0.25	

M3 = 0.998Sr + 0.002Eu; M6 = 0.998Sr + 0.002Eu

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

Experimental: powder, diffractometer, X-rays

Remarks: A similar structure was proposed for human tooth enamel in [2], where, however, CO<sub>3</sub> could not be located. Short interatomic distances for partly occupied site(s).

References: [1] Nötzold D., Wulff H. (1998), Phys. Status Solidi B 207, 271-282. [2] Young R.A., Mackie P.E. (1980), Mater. Res. Bull. 15, 17-29.