

$\text{K}(\text{La}_{0.5}\text{Pb}_{0.5})_2\text{F}_6$
hP15

(187) *P-6m2* – mleda

KLaPbF₆ [1]

Structural features: Infinite columns of base-linked (La,Pb)F₆F₃ tricapped trigonal prisms; disorder between two different arrangements with the prisms columns rotated by 60°.

Dib A. et al. (1987) [1]

F₆KLaPb

 $a = 0.6544$, $c = 0.3804$ nm, $c/a = 0.581$, $V = 0.1411$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	6 <i>m</i>	<i>m</i> ..	0.28033	0.02467	$\frac{1}{2}$	0.5	single atom F
F2	6 <i>l</i>	<i>m</i> ..	0.08733	0.41667	0	0.5	non-colinear F ₂
K3	1 <i>e</i>	-6 <i>m2</i>	$\frac{2}{3}$	$\frac{1}{3}$	0		coplanar hexagon F ₆
M4	1 <i>d</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		sixcapped hexagonal prism F ₁₈
M5	1 <i>a</i>	-6 <i>m2</i>	0	0	0		sixcapped hexagonal prism F ₁₈

 $\text{M4} = 0.5\text{La} + 0.5\text{Pb}$; $\text{M5} = 0.5\text{La} + 0.5\text{Pb}$

Transformation from published data: origin shift $\frac{2}{3}$ $\frac{1}{3}$ $\frac{1}{2}$

Experimental: twinned crystal, diffractometer, X-rays, $R = 0.032$

Remarks: Homogeneity range $\text{Pb}_{2x}\text{K}_{1.5-x}\text{La}_{1.5-x}\text{F}_6$, $0.3 < x < 0.6$. Average structure; the authors state that true symmetry may be space group (143) *P3* or (174) *P-6*.

References: [1] Dib A., Roux M.T., Aleonard S. (1987), J. Solid State Chem. 66, 47-55.