Table A1. Atomic coordinates, equivalent isotropic displacement parameters (Å^2), and occupancies for the sample La-K-Pym analyzed at 273(2) K.

Atom	*x*	*y*	*z*	U_{eq}	**Occ.**
Pb1	2/3	1/3	0.49478(4)	0.01495(6)	$Pb_{0.88(1)}La_{0.06(2)}K_{0.06(2)}$
Pb2	0.75085(2)	0.74497(2)	3/4	0.01481(4)	$Pb_{1.00}$
P	0.40974(13)	0.37862(13)	3/4	0.0086(2)	$P_{1.00}$
O1	0.3419(4)	0.4846(4)	3/4	0.0191(9)	$O_{1.00}$
O2	0.5893(4)	0.4743(4)	3/4	0.0167(9)	$O_{1.00}$
O3	0.3601(3)	0.2728(3)	0.5805(4)	0.0194(6)	$O_{1.00}$
Cl	1	1	1	0.0123(4)	$Cl_{1.00}$

Table A2. Experimental details and crystallographic characteristics of La-K-Pym analyzed at two different temperatures, 180(2) K and 273(2) K.

	La-K-Pym analyzed at 180(2) K*	La-K-Pym analyzed at 273(2) K
Diffractometer	Rigaku Oxford Diffraction	Bruker AXS
X-ray radiation	Mo*K*α (λ = 0.71073 Å)	Mo*K*α (λ = 0.71073 Å)
Temperature	180(2) K	273(2) K
Space group	$P6_3/m$	$P6_3/m$
Unit-cell parameters		
a (Å)	10.00129(8)	10.0011(5)
c (Å)	7.29865(8)	7.2986(5)
V (Å^3)	632.244(12)	632.22(8)
Z	2	2
Absorption coefficient	64.024 mm^{-1}	66.43 mm^{-1}
F(000)	1113	1132
θ range	2.35 to 33.78°	2.35 to 28.99°
Index ranges	-15<=h<=15, -15<=k<=15, -10<=l<=11	-13<=h<=13, -13<=k<=13, -9<=l<=9
Collected reflections / unique reflections	45590 / 893	7818 / 584
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Refined parameters	43	43
R1, Fo > 4sig(Fo)	0.0225	0.0165
R1, all unique data	0.0238	0.0184
wR2	0.0448	0.0351
GooF	1.189	1.175
Extinction coefficient	0.00006(7)	0.00018(4)
Largest difference peaks (e$^-$ Å^{-3})	4.679 and -1.960	3.065 and -1.008

** Data repeated in Table 2 and selected for discussion.*

Table A3. Comparison of selected bond lengths (Å), bond angles (°) and twist angles (°) for La-K-Pym analyzed at two different temperatures, 180(2) K and 273(2) K.

	La-K-Pym analyzed at 180(2) K*	La-K-Pym analyzed at 273(2) K
Pb1–O1 (×3)	2.581(4)	2.582(3)
O2 (×3)	2.674(4)	2.673(3)
O3 (×3)	2.881(5)	2.882(3)
Mean	2.712	2.712
Polyhedral volume (Å^3)	38.777	38.804
Pb2–O1	3.079(4)	3.074(3)
O2	2.356(6)	2.359(3)
O3 (×2)	2.625(4)	2.624(3)
O3 (×2)	2.636(5)	2.637(3)
Cl (×2)	3.1131(2)	3.11261(18)
Mean	2.773	2.773
Polyhedral volume (Å^3)	37.019	37.0037
P–O1	1.519(6)	1.518(4)
O2	1.557(6)	1.557(4)
O3 (×2)	1.539(4)	1.540(3)
Mean	1.536	1.539
Polyhedral volume (Å^3)	1.866	1.865
O1–P–O2	110.5(4)	110.6(2)
O1–P–O3 (×2)	112.3(2)	112.14(14)
O2–P–O3 (×2)	107.3(2)	107.40(14)
O3–P–O3	106.9(4)	106.9(2)
Twist angle	17.91	18.17

** Data repeated in Table 4 and selected for discussion.*