

Appendix D. Atomic coordinates, equivalent isotropic displacement parameters (\AA^2), and occupancies

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}	Occ.
Pb1					
La-Na-Pym	2/3	1/3	0.99498(4)	0.01428(13)	Pb _{0.810(9)} La _{0.090(9)} Na _{0.090(9)}
Na-Pym	1/3	2/3	0.50509(6)	0.01098(18)	Pb _{0.953(4)} Na _{0.047(4)}
La-K-Pym	2/3	1/3	0.00521(6)	0.01493(12)	Pb _{0.875(6)} La _{0.058(9)} K _{0.073(15)}
K-Pym	1/3	2/3	0.50519(6)	0.01293(16)	Pb _{0.932(4)} K _{0.068(4)}
Pb2					
La-Na-Pym	0.99437(2)	0.24912(3)	1/4	0.01529(9)	Pb _{1.00}
Na-Pym	0.24840(4)	0.25487(4)	1/4	0.01182(16)	Pb _{1.00}
La-K-Pym	0.00613(3)	0.25521(3)	1/4	0.01493(9)	Pb _{1.00}
K-Pym	0.24843(4)	0.25493(4)	1/4	0.01406(14)	Pb _{1.00}
P					
La-Na-Pym	0.03094(16)	0.40957(16)	3/4	0.0083(3)	P _{1.00}
Na-Pym	0.5901(3)	0.6212(2)	1/4	0.0054(4)	P _{1.00}
La-K-Pym	0.9691(2)	0.3787(2)	3/4	0.0085(3)	P _{1.00}
K-Pym	0.5901(2)	0.6212(2)	1/4	0.0077(4)	P _{1.00}
O1					
La-Na-Pym	0.8556(5)	0.3413(5)	3/4	0.0178(9)	O _{1.00}
Na-Pym	0.6575(8)	0.5142(8)	1/4	0.0134(13)	O _{1.00}
La-K-Pym	0.1429(7)	0.4850(7)	3/4	0.0197(12)	O _{1.00}
K-Pym	0.6574(8)	0.5142(8)	1/4	0.0170(14)	O _{1.00}
O2					
La-Na-Pym	0.5893(5)	0.4743(5)	1/4	0.0162(9)	O _{1.00}
Na-Pym	0.4101(8)	0.5257(8)	1/4	0.0130(13)	O _{1.00}
La-K-Pym	0.1149(7)	0.5255(7)	1/4	0.0180(11)	O _{1.00}
K-Pym	0.4098(7)	0.5250(7)	1/4	0.0151(13)	O _{1.00}
O3					
La-Na-Pym	0.0871(4)	0.3603(4)	0.9188(4)	0.0197(7)	O _{1.00}
Na-Pym	0.6395(6)	0.7269(6)	0.4189(7)	0.0151(10)	O _{1.00}
La-K-Pym	0.9127(5)	0.2729(5)	0.9194(6)	0.0199(8)	O _{1.00}
K-Pym	0.6396(6)	0.7267(5)	0.4190(7)	0.0173(9)	O _{1.00}
Cl					
La-Na-Pym	0	0	0	0.0145(4)	Cl _{1.00}
Na-Pym	0	0	0	0.0099(12)	Cl _{1.00}
La-K-Pym	0	0	0	0.0125(5)	Cl _{1.00}
K-Pym	0	0	0	0.0116(6)	Cl _{1.00}