Table 5. Positional parameters and B_{eq} ($Å^2$) with esd's in parentheses, of Pb-exchanged Poona, India sample.

atom	population	x/a	y/b	z/c	B_{eq}
T1		0.1796(4)	0.1695(3)	0.091(1)	1.04(8)*
T1'		-0.1778(4)	-0.1685(3)	-0.094(1)	1.01(8)*
T2		0.2874(4)	0.0894(3)	0.493(1)	0.98(8)*
T2'		-0.2839(4)	-0.0903(3)	-0.497(1)	1.38(9)*
T3		0.2961(4)	0.3081(3)	0.288(1)	1.03(8)*
T3'		-0.2895(4)	-0.3081(3)	-0.282(1)	1.04(8)*
T4		0.0670(4)	0.2991(3)	0.417(1)	0.94(8)*
T4'		-0.0634(4)	-0.3020(3)	-0.411(1)	1.10(8)*
T5		0	0.2160(2)	0	1.30(6)*
O1		0.299(1)	0	0.555(3)	2.40(4)*
O1'		0.199(1)	1/2	0.458(3)	2.20(4)*
O2		0.2351(9)	0.1248(8)	0.613(2)	2.50(3)*
O2'		-0.2238(9)	-0.1230(8)	-0.597(2)	2.60(3)*
O3		0.188(1)	0.1508(9)	-0.115(2)	3.20(3)*
O3'		-0.1807(9)	-0.1518(7)	0.117(2)	1.80(2)*
O4		0.231(1)	0.1017(9)	0.245(3)	3.20(3)*
O4'		-0.2389(8)	-0.1052(6)	-0.248(2)	1.20(2)*
O5		0	0.3280(6)	1/2	2.30(2)*
O6		0.082(1)	0.1623(9)	0.047(2)	2.90(3)*
O6'		-0.0824(7)	-0.1586(6)	-0.067(2)	1.20(2)*
O7		0.3807(9)	0.2654(8)	0.453(2)	2.50(3)*
O7'		-0.369(1)	-0.2632(8)	-0.442(2)	2.70(3)*

O8		0.0099(9)	0.2643(8)	0.194(2)	2.70(3)*
O8'		-0.0123(9)	-0.2743(8)	-0.183(2)	2.50(3)*
O9		0.2118(9)	0.2526(8)	0.178(2)	2.30(2)*
O9'		-0.2109(9)	-0.2522(8)	-0.171(2)	2.20(2)*
O10		0.1187(8)	0.3726(7)	0.401(2)	1.50(2)*
O10'		-0.118(1)	-0.3750(9)	-0.420(2)	3.30(3)*
PB1	0.318(4)	0.1505(5)	0	0.679(1)	5.40(1)
PB1'	0.404(4)	-0.1480(4)	0	-0.673(1)	4.40(8)
PB2'	0.608(3)	0.0381(3)	1/2	0.1979(9)	2.97(4)
PB3	0.144(4)	0.217(1)	0	0.877(3)	6.40(3)
PB3'	0.12(3)	-0.2060(8)	0	-0.860(3)	4.90(4)
PB4	0.144(6)	-0.011(1)	0.0768(9)	0.667(3)	12.7(4)
PB5	0.069(4)	0.009(3)	-0.100(2)	-0.516(6)	12.7(4)
O13		0.4218(8)	0.0873(8)	1.034(2)	2.90(3)
O22	0.76(5)	0.017(1)	0.074(1)	0.322(3)	2.00(5)*
O14		0.499(3)	0	0.502(7)	8.40(7)
O16'	0.88(4)	-0.076(2)	0	-0.879(6)	7.61(4)
O16	1.14(5)	0.077(2)	0	0.268(5)	9.29(6)
O27	0.6(4)	0.274(2)	0	-0.004(5)	2.20(9)*
O27'	0.86(6)	-0.276(2)	0	-0.018(4)	8.70(9)*
O28	0.22(3)	0.29(1)	0	0.25(2)	6.32*

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* Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as $B_{eq} = 8/3\ \pi^2\ \Sigma_i[\Sigma_j(\ U_{ij}\ a_i^*\ a_j^*\ a_i.aj)]$ Sigma(*Beq*): Schomaker, V. and Marsh, R.E. (1983) Acta Cryst A39, 819.

Warning: Sigmas(*Beq*) of atoms at special positions are not correct and may be too low by a factor up to 2.