

Table 3. Positional parameters and B_{eq} (\AA^2) with esd's in parentheses, of nonexchanged Poona, India sample.

atom	population	x/a	y/b	z/c	B_{eq}
T1		0.17940(8)	0.16975(8)	0.0967(2)	1.34(2)
T2		0.28859(8)	0.08989(8)	0.5008(2)	1.42(2)
T3		0.29172(8)	0.30959(8)	0.2831(2)	1.35(2)
T4		0.06460(8)	0.29843 (8)	0.4110(2)	1.34(2)
T5		0	0.2131(1)	0	1.40(3)
O1		0.3048(4)	0	0.5466(9)	2.80(1)
O2		0.2313(3)	0.1194(2)	0.6132(6)	3.05(7)
O3		0.1833(3)	0.1543(3)	-0.1158(6)	3.22(8)
O4		0.2385(2)	0.1065(2)	0.2555(6)	2.45(7)
O5		0	0.3259(3)	1/2	3.40(1)
O6		0.0820(2)	0.1587(2)	0.0626(6)	2.22(7)
O7		0.3729(3)	0.2660(3)	0.4508(6)	3.26(8)
O8		0.0089(3)	0.2662(3)	0.1842(6)	2.78(8)
O9		0.2103(2)	0.2542(2)	0.1783(6)	2.64(7)
O10		0.1155(2)	0.3723(2)	0.3988(6)	2.64(7)
Na1	1.108(8)	0.1549(3)	0	0.6666(7)	6.30(1)
Ca2	0.484(4)	0.5402(2)	0	0.2031(5)	2.74 (7)
K3	0.494(5)	0.2763(5)	0	0.010(1)	9.90(2)
O14		1/2	0	1/2	7.90(3)
O13		0.4228(3)	0.0817(3)	0.0307(9)	5.40(1)
O16		0.094(1)	0	0.285(3)	13.2(5)
O17	0.43(1)	0.082(1)	0.005(7)	0.867(3)	11.84 *

O19	0	0.0873(9)	1/2	20.5(8)
-----	---	-----------	-----	---------

* Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as $B_{eq} = 8/3 \pi^2 \sum_i [\sum_j (U_{ij} a_i^* a_j^* a_i \cdot a_j)]$
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.