

Table 4. Positional parameters and B_{eq} (\AA^2) with esd's in parentheses, of Na-exchanged Poona, India sample.

atom	population	x/a	y/b	z/c	B_{eq}
T1		0.17879(9)	0.16980(9)	0.0958(2)	1.49(3)
T2		0.28644(9)	0.08924(9)	0.4949(2)	1.53(3)
T3		0.29048(9)	0.30977(9)	0.2826(2)	1.52(2)
T4		0.06731(9)	0.29778(9)	0.4171(2)	1.52(3)
T5		0	0.2165(1)	0	1.60(4)
O1		0.3026(4)	0	0.5370(9)	2.40(1)
O2		0.2341(3)	0.1197(3)	0.6182(7)	3.23(8)
O3		0.1879(3)	0.1556(3)	-0.1090(7)	4.00(1)
O4		0.2311(3)	0.1033(3)	0.2498(6)	2.79(8)
O5		0	0.3218(4)	1/2	3.80(1)
O6		0.0807(3)	0.1609(3)	0.0493(7)	2.83(9)
O7		0.3737(3)	0.2686(3)	0.4492(7)	3.37(9)
O8		0.0145(3)	0.2709(3)	0.1862(7)	3.40(1)
O9		0.2123(3)	0.2521(3)	0.1875(7)	2.93(8)
O10		0.1199(3)	0.3719(3)	0.4212(7)	2.99(9)
Na1	0.80(2)	0.1726(7)	0	0.689(2)	10.3(3)
Na2	0.84(2)	0.5392(4)	0	0.243(1)	7.30(2)
Na3	0.84(2)	0.2839(9)	0	0.029(2)	16.1(4)
O14		1/2	0	1/2	13.6(6)
O13		0.4220(7)	0.0814(7)	0.035(2)	13.1(3)
O20	0.56(6)	0.074(4)	0	0.04(1)	26.9(34)*
O16		0.082(2)	0	0.271(6)	25.4(12)

O17	0.37(2)	0.072(2)	-0.029(2)	0.758(4)	11.84 *
O19		0	0.100(1)	1 / 2	22.20(9)

* 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(B_{eq}): Schomaker, V. and Marsh, R.E. (1983) Acta Cryst A39, 819.

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