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Table 4. Atom position and displacement parameters (run H4181)

Atom	$x/a$	$y/b$	$z/c$	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$	$U_{iso}$
M1	0	0	0	0.0076(3)	0.0060(2)	0.0076(3)	0	0	0	0.00707(19)
M2	0	0.25	0.97066(8)	0.0072(3)	0.0058(3)	0.0058(3)	0	0	0	0.0062(2)
M3	0.25	0.12617(3)	0.25	0.0067(2)	0.0078(3)	0.0073(2)	0	-0.00078(14)	0	0.00727(17)
T	0	0.12034(3)	0.61678(4)	0.0058(2)	0.0058(2)	0.0052(2)	0.00012(8)	0	0	0.00559(17)
O1	0	0.25	0.21814(16)	0.0046(5)	0.0059(5)	0.0064(6)	0	0	0	0.0056(2)
O2	0	0.25	0.71713(16)	0.0077(5)	0.0047(5)	0.0043(5)	0	0	0	0.0056(3)
O3	0	0.98891(8)	0.25591(11)	0.0063(3)	0.0059(4)	0.0044(4)	0.0009(3)	0	0	0.0056(2)
O4	0.26161(12)	0.12294(4)	0.99259(9)	0.0053(3)	0.0059(3)	0.0063(3)	0.00002(18)	0.0008(2)	-0.00011(13)	0.00585(19)