

Atom coordinate and isotropic thermal parameters of
serendibite (5151)

Table 3

	sof	x/a	y/b	z/c	$\bar{u}(\text{\AA})$
T1	0.627 B 0.373 Si	0.4650(2)	0.2353(2)	0.3293(2)	0.0064(4)
T2	1.0 Si	0.98384(8)	0.22747(8)	0.34077(8)	0.0069(2)
T3	1.0 Al	0.78592(9)	0.34431(9)	0.23325(9)	0.0053(2)
T4	0.983 B 0.017 Si	0.2704(3)	0.3300(3)	0.2194(3)	0.0065(7)
T5	1.0 Si	0.64424(9)	0.94387(9)	0.4431(9)	0.0087(2)
T6	1.0 Si	0.35632(8)	0.55453(8)	0.05409(8)	0.0059(2)
M1	1.0 Al	0	0	1/2	0.0041(3)
M2	0.936 Al 0.064 Fe	0	1/2	0	0.0051(3)
M3	0.907 Mg 0.093 Fe	0.31279(8)	0.85693(8)	0.17320(8)	0.0065(2)
M4	1.0 Al	0.77741(9)	0.82212(9)	0.14505(9)	0.0038(2)
M5	0.839 Mg 0.161 Fe	0.09511(8)	0.94434(8)	0.06202(8)	0.0060(2)
M6	0.910 Mg 0.090 Fe	0.59389(9)	0.93920(9)	0.05777(9)	0.0054(2)
M7	1.0 Al	0.99809(9)	0.74093(8)	0.25915(8)	0.0035(2)
M8	1.0 Ca	0.21468(7)	0.62410(6)	0.39752(6)	0.0095(2)
M9	1.0 Ca	0.64819(6)	0.60210(6)	0.38268(6)	0.0107(2)
O1	1.0	0.3531(2)	0.0648(2)	0.1719(2)	0.0107(6)
O2	1.0	0.8437(2)	0.0481(2)	0.1670(2)	0.0094(5)
O3	1.0	0.5415(2)	0.9546(2)	0.2874(2)	0.0143(6)
O4	1.0	0.0143(2)	0.9342(2)	0.2768(2)	0.0084(5)
O5	1.0	0.2396(2)	0.8662(2)	0.3812(2)	0.0097(5)
O6	1.0	0.7632(2)	0.8810(2)	0.3826(2)	0.0086(5)
O7	1.0	0.4903(2)	0.2100(2)	0.4947(2)	0.0120(6)
O8	1.0	0.9566(2)	0.7881(2)	0.4816(2)	0.0087(5)
O9	1.0	0.9000(2)	0.3269(2)	0.3803(2)	0.0096(5)

O10	1.0	0.3851(2)	0.3276(2)	0.3454(2)	0.0093(5)
O11	1.0	0.6514(2)	0.1637(2)	0.0482(2)	0.0102(5)
O12	1.0	0.1617(2)	0.1773(2)	0.0629(2)	0.0089(5)
O13	1.0	0.5372(2)	0.7111(2)	0.0485(2)	0.0111(5)
O14	1.0	0.0681(2)	0.7261(2)	0.0640(2)	0.0087(5)
O15	1.0	0.2405(2)	0.6153(2)	0.1172(2)	0.0087(5)
O16	1.0	0.7527(2)	0.6132(2)	0.1351(2)	0.0100(5)
O17	1.0	0.3902(2)	0.4875(2)	0.1933(2)	0.0080(5)
O18	1.0	0.9509(2)	0.5252(2)	0.2160(2)	0.0103(5)
O19	1.0	0.1670(2)	0.3602(2)	0.3131(2)	0.0098(5)
O20	1.0	0.6576(2)	0.3691(2)	0.3343(2)	0.0124(6)

Note :

sof = site occupancy factors. $\bar{u}$ = isotropic temperature factor
Standard deviations of the last digit are in parentheses.

Atom coordinate and isotropic thermal parameters of
serendibite (5152)

Table 3

	sof	x/a	y/b	z/c	$\bar{u}(\text{\AA})$
T1	0.493 B 0.507 Si	0.4655(1)	0.2358(1)	0.3297(1)	0.007(1)
T2	1.0 Si	0.9841(1)	0.2282(1)	0.3409(1)	0.0083(7)
T3	1.0 Al	0.7871(1)	0.3450(1)	0.2342(1)	0.0063(7)
T4	0.966 B 0.034 Si	0.2698(3)	0.3318(3)	0.2207(3)	0.007(2)
T5	1.0 Si	0.6444(1)	0.9446(1)	0.4423(1)	0.0098(7)
T6	1.0 Si	0.3559(1)	0.5543(1)	0.0539(1)	0.0073(7)
M1	0.943 Al 0.057 Fe	0	0	1/2	0.006(1)
M2	0.836 Al 0.164 Fe	0	1/2	0	0.006(1)
M3	0.804 Al 0.196 Fe	0.3131(1)	0.8564(1)	0.1727(1)	0.0074(7)
M4	0.851 Al 0.149 Fe	0.7766(1)	0.8217(1)	0.1445(1)	0.0076(7)
M5	0.687 Mg 0.313 Fe	0.0940(1)	0.9430(1)	0.0609(1)	0.0076(7)
M6	0.787 Mg 0.213 Fe	0.5944(1)	0.9401(1)	0.0593(1)	0.0075(7)
M7	0.909 Al 0.091 Fe	0.9981(1)	0.7409(1)	0.2594(1)	0.0056(7)
M8	1.0 Ca	0.21353(9)	0.62396(9)	0.39671(7)	0.0110(5)
M9	1.0 Ca	0.64845(10)	0.60299(7)	0.38105(7)	0.0122(6)
O1	1.0	0.3518(2)	0.0634(2)	0.1700(2)	0.012(2)
O2	1.0	0.8443(2)	0.0408(2)	0.1678(2)	0.010(2)
O3	1.0	0.5427(2)	0.9561(2)	0.2871(2)	0.015(2)
O4	1.0	0.0148(2)	0.9342(2)	0.2772(2)	0.009(2)
O5	1.0	0.2394(2)	0.8659(2)	0.3822(2)	0.010(2)
O6	1.0	0.7629(2)	0.8809(2)	0.3831(2)	0.011(2)
O7	1.0	0.4918(2)	0.2095(2)	0.4872(2)	0.014(2)

O8	1.0	0.9558(2)	0.7874(2)	0.4821(2)	0.010(2)
O9	1.0	0.9001(2)	0.3269(2)	0.3804(2)	0.011(2)
O10	1.0	0.3849(2)	0.3304(2)	0.3470(2)	0.012(2)
O11	1.0	0.6517(2)	0.1648(2)	0.0504(2)	0.011(2)
O12	1.0	0.1622(2)	0.1780(2)	0.0643(2)	0.011(2)
O13	1.0	0.5362(2)	0.7107(2)	0.0487(2)	0.012(2)
O14	1.0	0.0676(2)	0.7254(2)	0.0637(2)	0.010(2)
O15	1.0	0.2409(2)	0.6156(2)	0.1175(2)	0.010(2)
O16	1.0	0.7524(2)	0.6123(2)	0.1353(2)	0.011(2)
O17	1.0	0.3895(2)	0.4873(2)	0.1925(2)	0.009(2)
O18	1.0	0.9511(2)	0.5251(2)	0.2163(2)	0.012(2)
O19	1.0	0.1660(2)	0.3613(2)	0.3123(2)	0.012(2)
O20	1.0	0.6606(2)	0.3724(2)	0.3358(2)	0.014(2)

Note :

sof = site occupancy factor, $\bar{u}$ = isotropic temperature factor.
Standard deviations of the last digit are in parentheses.