Table 5. Atomic fractional coordinates and equivalent displacement parameters

Atom	x	y	z	Beq(Å^2)
Ca	0.000	0.30155(2)	0.250	0.592(2)
Mg	0.000	0.90833(3)	0.250	0.425(4)
Si	0.28621(2)	0.09328(2)	0.22933(3)	0.343(2)
O1	0.11559(4)	0.08748(5)	0.14242(9)	0.482(6)
O2	0.36128(5)	0.24995(5)	0.31853(8)	0.618(6)
O3	0.35070(4)	0.01793(5)	0.99526(8)	0.543(6)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3)[a^2ß(1,1) + b^2ß(2,2) + c^2ß(3,3) + ab(\cos\gamma)ß(1,2) + ac(\cos\beta)ß(1,3) + bc(\cos\alpha)ß(2,3)]$

Table 6: General displacement parameter expressions - U's

Atom	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Ca	0.00957(5)	0.00587(5)	0.00581(5)	0	-0.00002(4)	0
Mg	0.00611(8)	0.0054(1)	0.00448(9)	0	0.00112(7)	0
Si	0.00430(5)	0.00476(6)	0.00395(5)	-0.00023(4)	0.00106(4)	-0.00017(4)
O1	0.0047(1)	0.0071(1)	0.0064(1)	-0.0001(1)	0.0012(1)	-0.0000(1)
O2	0.0094(1)	0.0067(2)	0.0070(1)	-0.0023(1)	0.0018(1)	-0.0006(1)
O3	0.0065(1)	0.0090(2)	0.0053(1)	-0.0001(1)	0.0018(1)	-0.0018(1)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2\{h^2a^{*2}U(1,1)+k^2b^{*2}U(2,2)+l^2c^{*2}U(3,3)+2hka^*b^*U(1,2)+2hla^*c^*U(1,3) + 2klb^*c^*U(2,3)\}]$ where a^*, b^*, and c^* are reciprocal lattice constants.