Table 5. Atomic fractional coordinates and equivalent displacement parameters

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>Beq(Å²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca</td>
<td>0.000</td>
<td>0.30155(2)</td>
<td>0.250</td>
<td>0.592(2)</td>
</tr>
<tr>
<td>Mg</td>
<td>0.000</td>
<td>0.90833(3)</td>
<td>0.250</td>
<td>0.425(4)</td>
</tr>
<tr>
<td>Si</td>
<td>0.28621(2)</td>
<td>0.09328(2)</td>
<td>0.22933(3)</td>
<td>0.343(2)</td>
</tr>
<tr>
<td>O1</td>
<td>0.11559(4)</td>
<td>0.08748(5)</td>
<td>0.14242(9)</td>
<td>0.482(6)</td>
</tr>
<tr>
<td>O2</td>
<td>0.36128(5)</td>
<td>0.24995(5)</td>
<td>0.31853(8)</td>
<td>0.618(6)</td>
</tr>
<tr>
<td>O3</td>
<td>0.35070(4)</td>
<td>0.01793(5)</td>
<td>0.99526(8)</td>
<td>0.543(6)</td>
</tr>
</tbody>
</table>

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

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

Table 6: General displacement parameter expressions - U’s

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

The form of the anisotropic displacement parameter is:

\[\exp[-2\pi^2\{h^2a^*{}^2U(1,1)+k^2b^*{}^2U(2,2)+l^2c^*{}^2U(3,3)+2hkab^*{}^2U(1,2)+2hla^*{}^2U(1,3)+2klb^*{}^2U(2,3)\}]

where \(a^*, b^*,\) and \(c^*\) are reciprocal lattice constants.