Table 1b. The fractional coordinates of the oxygen atoms ($\times 10^3$) and isotropic temperature factors (those from D11 down to U66 are equivalent temperature factors)

<table>
<thead>
<tr>
<th>Site</th>
<th>Occu-</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>B(Å²)</th>
<th>Site</th>
<th>Occu-</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>B(Å²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1A</td>
<td>0.5</td>
<td>990(3)</td>
<td>0</td>
<td>245(5)</td>
<td>4.2(8)</td>
<td>U95</td>
<td>0.32</td>
<td>212</td>
<td>0</td>
<td>681</td>
<td>1.3(3)</td>
</tr>
<tr>
<td>1B</td>
<td>0.5</td>
<td>988(3)</td>
<td>0</td>
<td>245(5)</td>
<td>4.2(8)</td>
<td>U96</td>
<td>0.32</td>
<td>141</td>
<td>189</td>
<td>627</td>
<td>1.3(3)</td>
</tr>
<tr>
<td>2A</td>
<td>0.5</td>
<td>038(3)</td>
<td>0</td>
<td>119(4)</td>
<td>3.8(11)</td>
<td>G91</td>
<td>0.045</td>
<td>140</td>
<td>050</td>
<td>584</td>
<td>1.3(3)</td>
</tr>
<tr>
<td>2B</td>
<td>0.5</td>
<td>052(3)</td>
<td>0</td>
<td>124(5)</td>
<td>3.8(11)</td>
<td>G92</td>
<td>0.045</td>
<td>133</td>
<td>-123</td>
<td>712</td>
<td>1.3(3)</td>
</tr>
<tr>
<td>3A</td>
<td>0.5</td>
<td>030(2)</td>
<td>0</td>
<td>599(3)</td>
<td>2.8(9)</td>
<td>G93</td>
<td>0.045</td>
<td>204</td>
<td>-123</td>
<td>655</td>
<td>1.3(3)</td>
</tr>
<tr>
<td>3B</td>
<td>0.5</td>
<td>038(2)</td>
<td>0</td>
<td>610(4)</td>
<td>2.8(9)</td>
<td>G94</td>
<td>0.045</td>
<td>175</td>
<td>197</td>
<td>706</td>
<td>1.3(3)</td>
</tr>
<tr>
<td>4A</td>
<td>0.5</td>
<td>-004(2)</td>
<td>0</td>
<td>753(3)</td>
<td>1.0(3)</td>
<td>D101</td>
<td>0.59</td>
<td>255</td>
<td>0</td>
<td>335</td>
<td>11(4)</td>
</tr>
<tr>
<td>4B</td>
<td>0.5</td>
<td>-003(2)</td>
<td>0</td>
<td>754(3)</td>
<td>1.0(3)</td>
<td>D102</td>
<td>0.59</td>
<td>268</td>
<td>0</td>
<td>480</td>
<td>2.7(8)</td>
</tr>
<tr>
<td>5A</td>
<td>0.5</td>
<td>372(2)</td>
<td>0</td>
<td>-077(3)</td>
<td>2.8(9)</td>
<td>D103</td>
<td>0.59</td>
<td>206</td>
<td>189</td>
<td>415</td>
<td>2.0(5)</td>
</tr>
<tr>
<td>5B</td>
<td>0.5</td>
<td>373(2)</td>
<td>0</td>
<td>-074(4)</td>
<td>2.8(9)</td>
<td>U104</td>
<td>0.41</td>
<td>212</td>
<td>0</td>
<td>487</td>
<td>6(3)</td>
</tr>
<tr>
<td>6A</td>
<td>0.5</td>
<td>329(3)</td>
<td>0</td>
<td>075(4)</td>
<td>4.1(8)</td>
<td>U105</td>
<td>0.41</td>
<td>283</td>
<td>0</td>
<td>430</td>
<td>2(1)</td>
</tr>
<tr>
<td>6B</td>
<td>0.5</td>
<td>331(3)</td>
<td>0</td>
<td>077(5)</td>
<td>4.1(8)</td>
<td>U106</td>
<td>0.41</td>
<td>221</td>
<td>189</td>
<td>365</td>
<td>3(1)</td>
</tr>
<tr>
<td>7A</td>
<td>0.5</td>
<td>289(2)</td>
<td>0</td>
<td>211(4)</td>
<td>2.7(7)</td>
<td>D111</td>
<td>0.57</td>
<td>444</td>
<td>0</td>
<td>175</td>
<td>5(2)</td>
</tr>
<tr>
<td>7B</td>
<td>0.5</td>
<td>289(2)</td>
<td>0</td>
<td>223(4)</td>
<td>2.7(7)</td>
<td>D112</td>
<td>0.57</td>
<td>372</td>
<td>0</td>
<td>233</td>
<td>3(1)</td>
</tr>
<tr>
<td>8A</td>
<td>0.5</td>
<td>362(1)</td>
<td>0</td>
<td>441(2)</td>
<td>0.8(3)</td>
<td>D113</td>
<td>0.57</td>
<td>435</td>
<td>189</td>
<td>298</td>
<td>3(1)</td>
</tr>
<tr>
<td>8B</td>
<td>0.5</td>
<td>362(1)</td>
<td>0</td>
<td>442(2)</td>
<td>0.8(3)</td>
<td>U114</td>
<td>0.43</td>
<td>399</td>
<td>0</td>
<td>327</td>
<td>5(2)</td>
</tr>
<tr>
<td>9A</td>
<td>0.5</td>
<td>325(1)</td>
<td>0</td>
<td>583(2)</td>
<td>0.1(4)</td>
<td>U115</td>
<td>0.43</td>
<td>382</td>
<td>0</td>
<td>193</td>
<td>5(2)</td>
</tr>
<tr>
<td>9B</td>
<td>0.5</td>
<td>334(1)</td>
<td>0</td>
<td>595(2)</td>
<td>0.1(4)</td>
<td>U116</td>
<td>0.43</td>
<td>450</td>
<td>189</td>
<td>257</td>
<td>2.3(8)</td>
</tr>
<tr>
<td>10A</td>
<td>0.5</td>
<td>282(1)</td>
<td>0</td>
<td>724(3)</td>
<td>1.4(5)</td>
<td>U124</td>
<td>0.43</td>
<td>478</td>
<td>0</td>
<td>080</td>
<td>6(1)</td>
</tr>
<tr>
<td>10B</td>
<td>0.5</td>
<td>293(2)</td>
<td>0</td>
<td>732(3)</td>
<td>1.4(5)</td>
<td>U125</td>
<td>0.43</td>
<td>550</td>
<td>0</td>
<td>022</td>
<td>6(1)</td>
</tr>
<tr>
<td>11A</td>
<td>0.5</td>
<td>666(1)</td>
<td>0</td>
<td>-093(2)</td>
<td>0.5(4)</td>
<td>U126</td>
<td>0.43</td>
<td>487</td>
<td>189</td>
<td>043</td>
<td>6(1)</td>
</tr>
<tr>
<td>11B</td>
<td>0.5</td>
<td>675(1)</td>
<td>0</td>
<td>-081(2)</td>
<td>0.5(4)</td>
<td>G121</td>
<td>0.285</td>
<td>478</td>
<td>050</td>
<td>-075</td>
<td>6(1)</td>
</tr>
<tr>
<td>12A</td>
<td>0.5</td>
<td>627(2)</td>
<td>0</td>
<td>049(3)</td>
<td>1.5(6)</td>
<td>G122</td>
<td>0.285</td>
<td>466</td>
<td>-123</td>
<td>040</td>
<td>6(1)</td>
</tr>
<tr>
<td>12B</td>
<td>0.5</td>
<td>634(2)</td>
<td>0</td>
<td>067(3)</td>
<td>1.5(6)</td>
<td>G123</td>
<td>0.285</td>
<td>542</td>
<td>-123</td>
<td>-004</td>
<td>6(1)</td>
</tr>
<tr>
<td>13A</td>
<td>0.5</td>
<td>706(2)</td>
<td>0</td>
<td>285(4)</td>
<td>2.6(6)</td>
<td>G124</td>
<td>0.285</td>
<td>513</td>
<td>197</td>
<td>047</td>
<td>6(1)</td>
</tr>
<tr>
<td>13B</td>
<td>0.5</td>
<td>704(2)</td>
<td>0</td>
<td>290(4)</td>
<td>2.6(6)</td>
<td>D131</td>
<td>0.37</td>
<td>520</td>
<td>0</td>
<td>425</td>
<td>3.4(6)</td>
</tr>
<tr>
<td>14A</td>
<td>0.5</td>
<td>648(2)</td>
<td>0</td>
<td>421(3)</td>
<td>2.1(7)</td>
<td>D132</td>
<td>0.37</td>
<td>448</td>
<td>0</td>
<td>483</td>
<td>3.4(6)</td>
</tr>
<tr>
<td>14B</td>
<td>0.5</td>
<td>655(2)</td>
<td>0</td>
<td>414(3)</td>
<td>2.1(7)</td>
<td>D133</td>
<td>0.37</td>
<td>511</td>
<td>189</td>
<td>547</td>
<td>3.4(6)</td>
</tr>
<tr>
<td>15A</td>
<td>0.5</td>
<td>608(1)</td>
<td>0</td>
<td>564(3)</td>
<td>1.5(6)</td>
<td>G131</td>
<td>0.315</td>
<td>520</td>
<td>050</td>
<td>580</td>
<td>3.4(6)</td>
</tr>
<tr>
<td>15B</td>
<td>0.5</td>
<td>622(2)</td>
<td>0</td>
<td>567(3)</td>
<td>1.5(6)</td>
<td>G132</td>
<td>0.315</td>
<td>526</td>
<td>-128</td>
<td>451</td>
<td>3.4(6)</td>
</tr>
<tr>
<td>16A</td>
<td>0.5</td>
<td>705(1)</td>
<td>0</td>
<td>763(3)</td>
<td>1.4(5)</td>
<td>G133</td>
<td>0.315</td>
<td>456</td>
<td>-123</td>
<td>308</td>
<td>3.4(6)</td>
</tr>
<tr>
<td>16B</td>
<td>0.5</td>
<td>706(2)</td>
<td>0</td>
<td>771(3)</td>
<td>1.4(5)</td>
<td>G134</td>
<td>0.315</td>
<td>463</td>
<td>197</td>
<td>463</td>
<td>3.4(6)</td>
</tr>
<tr>
<td>17A</td>
<td>0.5</td>
<td>947(2)</td>
<td>0</td>
<td>401(3)</td>
<td>1.5(6)</td>
<td>D141</td>
<td>0.37</td>
<td>591</td>
<td>0</td>
<td>629</td>
<td>16(9)</td>
</tr>
<tr>
<td>17B</td>
<td>0.5</td>
<td>957(2)</td>
<td>0</td>
<td>401(3)</td>
<td>1.5(6)</td>
<td>D142</td>
<td>0.37</td>
<td>591</td>
<td>0</td>
<td>629</td>
<td>16(9)</td>
</tr>
</tbody>
</table>