TABLE SM 1:
Force constants ,C_i, of O-C-O in dimensionless normal
coordinates (in wavenumbers).

<table>
<thead>
<tr>
<th>i</th>
<th>i1</th>
<th>i2</th>
<th>i3</th>
<th>Ci</th>
<th>Ci1</th>
<th>Ci2</th>
<th>Ci3</th>
<th>CCSD(T)</th>
<th>DFT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>1198.888</td>
<td>1198.118</td>
<td>1179.435</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>677.165</td>
<td>675.922</td>
<td>661.126</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>2</td>
<td>0</td>
<td>-252.351</td>
<td>-251.682</td>
<td>-247.605</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>4</td>
<td>0</td>
<td>6.598</td>
<td>6.769</td>
<td>6.752</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>-43.019</td>
<td>-44.524</td>
<td>-43.672</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>19.428</td>
<td>20.653</td>
<td>20.814</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>1</td>
<td>4</td>
<td>0</td>
<td>?</td>
<td>-1.149</td>
<td>-0.879</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0</td>
<td>6</td>
<td>0</td>
<td>0.068</td>
<td>0.012</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>4</td>
<td>0</td>
<td>0</td>
<td>1.407</td>
<td>1.770</td>
<td>1.778</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>3</td>
<td>2</td>
<td>0</td>
<td>4.119</td>
<td>-1.104</td>
<td>-0.880</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>2</td>
<td>4</td>
<td>0</td>
<td>-1.540</td>
<td>0.073</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>5</td>
<td>0</td>
<td>0</td>
<td>?</td>
<td>-0.047</td>
<td>-0.045</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>4</td>
<td>2</td>
<td>0</td>
<td>1.185</td>
<td>0.037</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>336.330</td>
<td>335.434</td>
<td>321.211</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>75.369</td>
<td>75.559</td>
<td>77.299</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>0</td>
<td>2</td>
<td>1</td>
<td>-28.165</td>
<td>-27.703</td>
<td>-27.348</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>-11.188</td>
<td>-11.763</td>
<td>-11.650</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>5.400</td>
<td>5.586</td>
<td>5.947</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>0</td>
<td>4</td>
<td>1</td>
<td>-0.187</td>
<td>-0.194</td>
<td>-0.173</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>3</td>
<td>0</td>
<td>1</td>
<td>0.665</td>
<td>0.823</td>
<td>0.894</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>0.397</td>
<td>-0.524</td>
<td>-0.471</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>1</td>
<td>4</td>
<td>1</td>
<td>?</td>
<td>0.026</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>4</td>
<td>0</td>
<td>1</td>
<td>-0.885</td>
<td>-0.031</td>
<td>-0.039</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>3</td>
<td>2</td>
<td>1</td>
<td>?</td>
<td>0.023</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>2.587</td>
<td>2.751</td>
<td>3.363</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>-1.052</td>
<td>-1.049</td>
<td>-0.864</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>0</td>
<td>2</td>
<td>2</td>
<td>0.313</td>
<td>0.283</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>2</td>
<td>0</td>
<td>2</td>
<td>0.097</td>
<td>0.129</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>?</td>
<td>-0.054</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>0</td>
<td>4</td>
<td>2</td>
<td>?</td>
<td>0.002</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>31</td>
<td>3</td>
<td>0</td>
<td>2</td>
<td>?</td>
<td>-0.008</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>?</td>
<td>0.004</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>33</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>?</td>
<td>-0.024</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>34</td>
<td>1</td>
<td>0</td>
<td>3</td>
<td>?</td>
<td>0.006</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>0</td>
<td>2</td>
<td>3</td>
<td>?</td>
<td>-0.001</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>2</td>
<td>0</td>
<td>3</td>
<td>?</td>
<td>-0.001</td>
<td>?</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
\[ V = \sum_i \{ C_i q_1^{i_1} q_2^{i_2} (q_3a^2 + q_3b^2)^{i_3} \} \]


This study.

*******************************************************************************
*******************************************************************************

### TABLE SM 2:
Valence force constants, \( C_i \), of O-C-O-K+ in the curvilinear coordinates (in units providing \( V \) in wavenumbers)

<table>
<thead>
<tr>
<th>i</th>
<th>i1</th>
<th>i2</th>
<th>i3</th>
<th>i4</th>
<th>i5</th>
<th>C_i</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>414269.453</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>52957.829</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>4526.592</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-368708.055</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>-4906.581</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-970691.799</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>i</th>
<th>i1</th>
<th>i2</th>
<th>i3</th>
<th>i4</th>
<th>i5</th>
<th>C_i</th>
</tr>
</thead>
<tbody>
<tr>
<td>27</td>
<td>4</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>130235.298</td>
</tr>
<tr>
<td>28</td>
<td>2</td>
<td>0</td>
<td>3</td>
<td>0</td>
<td>0</td>
<td>10067.144</td>
</tr>
<tr>
<td>29</td>
<td>0</td>
<td>5</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-1104801.201</td>
</tr>
<tr>
<td>30</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>17726.004</td>
</tr>
<tr>
<td>31</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>-27082.049</td>
</tr>
<tr>
<td>32</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>-26168.103</td>
</tr>
<tr>
<td>33</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>0</td>
<td>294.377</td>
</tr>
</tbody>
</table>

\[ V = \sum_i \{ C_i \cdot (R_{OC} - 1.158123)^i1 \cdot (R_{CO} - 1.181405)^i2 \cdot (R_{OK} - 2.678163)^i3 \cdot \gamma_x^i4 \cdot \chi_x^i5 \} \]