Hydrogen-bonded intermediate and transition states during spontaneous and acid-catalyzed hydrolysis of the carcinogen (+)-anti-BPDE

Mark C. Palenik, Jorge H. Rodriguez,∗a

Supplementary material

aTheoretical and Computational Biomolecular Physics Group, Department of Physics and Astronomy, Purdue University, West Lafayette, IN, 47907, USA.

*corresponding author, E-mail: jhrodrig@purdue.edu
Activation barriers of Table were calculated in this work based on their corresponding experimental (kinetic) data \([1,2]\) using the formula

\[
k = \frac{k_B T}{\epsilon^0 h} e^{-\Delta G^\ddagger / k_B T}
\]

which was inverted to find \(\Delta G^\ddagger\) in terms of \(k\), where \(k\) is the reaction rate, \(\epsilon^0\) is the standard concentration of 1 M, \(k_B\) is Boltzmann’s constant, and \(h\) is Planck’s constant.

The computationally determined values of \(\Delta G^\ddagger\) reproduced the main trends of the experimental values and, at the same time, were somewhat higher than these. With the 6-311g* basis set, the error was around 1-5 kcal mol\(^{-1}\) for cacodylic acid catalyzed hydrolysis and 5-10 kcal mol\(^{-1}\) for spontaneous hydrolysis. The error was slightly larger with the 6-311+g* basis set, possibly because of the interaction of the extra diffuse orbitals with the implicit solvation model. In both cases, spontaneous and acid catalized, the BLYP/6-311g* and BLYP/6-311+g* functional/basis set combination (displayed in bold in Table ) produced the best agreement with experiment.
Table S3: Energies of HB...BPDE relative to those of non-interacting (+)-anti-BPDE and cacodylic acid in the solvent phase [kcal mol\(^{-1}\)].

<table>
<thead>
<tr>
<th></th>
<th>6-311g*</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ε\text{KS}</td>
<td>ΔΖ</td>
<td>ΔΗ</td>
</tr>
<tr>
<td>BPW91</td>
<td>-6.92</td>
<td>1.31</td>
</tr>
<tr>
<td>BLYP</td>
<td>-8.96</td>
<td>1.31</td>
</tr>
<tr>
<td>B1LYP</td>
<td>-9.47</td>
<td>1.29</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-9.44</td>
<td>1.22</td>
</tr>
</tbody>
</table>

Includes −1.89 kcal/mol correction to entropy and free energy to account for change in standard conditions in the gas phase to standard conditions in the solvated phase.

Table S4: Energies of H\(_2\)O...BPDE relative to those of its non-interacting components in the solvent phase [kcal mol\(^{-1}\)].

<table>
<thead>
<tr>
<th></th>
<th>6-311g*</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Ε\text{KS}</td>
<td>ΔΖ</td>
<td>ΔΗ</td>
</tr>
<tr>
<td>BPW91</td>
<td>-4.42</td>
<td>1.70</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-6.01</td>
<td>1.86</td>
</tr>
</tbody>
</table>

Includes −1.89 kcal/mol correction to entropy and free energy to account for change in standard conditions in the gas phase to standard conditions in the solvated phase.

Table contains the computed energies of the hydrogen bonded HB...BPDE complex relative to its separate components (Fig. 4). The negative value of Ε\text{KS} indicates that the hydrogen bond has the effect of lowering the electronic energy of the system. ΔG is positive because the hydrogen bond also corresponds to a decrease in entropy of the entire complex, and thus the Gibbs free energy of the hydrogen bonded complex is between that of the separate components and the transition state. This result holds for both the gas phase and solvated calculations.

If the hydrogen bonded structure were at a Gibbs free energy lower than that corresponding to the sum of the individual reactants and if it forms before an chemical (as opposed to non-covalent) process takes place, this would correspond to an increase in the activation barrier. However, the decrease in enthalpy of the hydrogen bonded complex is more than compensated by a concomitant decrease in entropy.

When water acts as the proton donor, a hydrogen bonded structure can also be found (H\(_2\)O...BPDE) where water is interacting with O3 (Fig. 3). Table contains the energies of the water/BPDE hydrogen bonded complex relative to the sum of those corresponding to its non-interacting components.
Table S5: $\Delta G$ for BPDE hydrolysis [kcal mol$^{-1}$].

<table>
<thead>
<tr>
<th>Method</th>
<th>$\Delta E^*$</th>
<th>$\Delta Z$</th>
<th>$\Delta H$</th>
<th>$-T\Delta S$</th>
<th>$\Delta G$</th>
<th>$\Delta E^*$</th>
<th>$\Delta Z$</th>
<th>$\Delta H$</th>
<th>$-T\Delta S$</th>
<th>$\Delta G$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>-18.09</td>
<td>3.70</td>
<td>-15.38</td>
<td>10.64</td>
<td>-4.74</td>
<td>-14.36</td>
<td>3.43</td>
<td>-11.80</td>
<td>10.27</td>
<td>-1.53</td>
</tr>
<tr>
<td>BLYP</td>
<td>-19.36</td>
<td>3.79</td>
<td>-16.57</td>
<td>10.61</td>
<td>-5.96</td>
<td>-14.71</td>
<td>3.55</td>
<td>-12.06</td>
<td>10.40</td>
<td>-1.66</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-22.34</td>
<td>3.92</td>
<td>-19.45</td>
<td>10.62</td>
<td>-8.82</td>
<td>-18.31</td>
<td>3.73</td>
<td>-15.53</td>
<td>10.44</td>
<td>-5.09</td>
</tr>
</tbody>
</table>

Table S6: Energies for BPDE-Cacodylic acid hydrogen bonded structure HB...BPDE [Hartrees].

<table>
<thead>
<tr>
<th>Method</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>-3463.284512</td>
<td>0.372636</td>
<td>0.400244</td>
<td>0.315383</td>
<td>-3463.310438</td>
<td>0.371251</td>
<td>0.399261</td>
<td>0.312014</td>
</tr>
<tr>
<td>BLYP</td>
<td>-3462.855784</td>
<td>0.370282</td>
<td>0.398040</td>
<td>0.312854</td>
<td>-3462.886833</td>
<td>0.36927</td>
<td>0.397116</td>
<td>0.309399</td>
</tr>
<tr>
<td>B1LYP</td>
<td>-3462.651524</td>
<td>0.385137</td>
<td>0.411950</td>
<td>0.328501</td>
<td>-3462.678735</td>
<td>0.384032</td>
<td>0.411112</td>
<td>0.326260</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-3463.280469</td>
<td>0.382855</td>
<td>0.409868</td>
<td>0.325415</td>
<td>-3463.307736</td>
<td>0.381941</td>
<td>0.409129</td>
<td>0.324216</td>
</tr>
</tbody>
</table>

Table S7: Energies for $\text{(+)}$-anti-BPDE [Hartrees].

<table>
<thead>
<tr>
<th>Method</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>-996.337613</td>
<td>0.281862</td>
<td>0.299739</td>
<td>0.238315</td>
<td>-996.356405</td>
<td>0.281307</td>
<td>0.299311</td>
<td>0.237736</td>
</tr>
<tr>
<td>BLYP</td>
<td>-996.090562</td>
<td>0.279969</td>
<td>0.297887</td>
<td>0.236482</td>
<td>-996.113028</td>
<td>0.279548</td>
<td>0.297606</td>
<td>0.235946</td>
</tr>
<tr>
<td>B1LYP</td>
<td>-995.959720</td>
<td>0.291546</td>
<td>0.308741</td>
<td>0.248693</td>
<td>-995.979432</td>
<td>0.290106</td>
<td>0.308351</td>
<td>0.248034</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-996.449192</td>
<td>0.289861</td>
<td>0.307206</td>
<td>0.246959</td>
<td>-996.469152</td>
<td>0.289271</td>
<td>0.306777</td>
<td>0.246149</td>
</tr>
</tbody>
</table>

Table S8: Energies for $\text{H}_2\text{O}$ [Hartrees].

<table>
<thead>
<tr>
<th>Method</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>-76.433735</td>
<td>0.020784</td>
<td>0.024563</td>
<td>0.003114</td>
<td>-76.444243</td>
<td>0.020672</td>
<td>0.024451</td>
<td>0.003002</td>
</tr>
<tr>
<td>BLYP</td>
<td>-76.423750</td>
<td>0.020546</td>
<td>0.024325</td>
<td>0.002865</td>
<td>-76.436796</td>
<td>0.020442</td>
<td>0.024221</td>
<td>0.002762</td>
</tr>
<tr>
<td>B1LYP</td>
<td>-76.411126</td>
<td>0.021426</td>
<td>0.025205</td>
<td>0.003875</td>
<td>-76.421795</td>
<td>0.021315</td>
<td>0.025094</td>
<td>0.003674</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-76.442572</td>
<td>0.021308</td>
<td>0.025087</td>
<td>0.003663</td>
<td>-76.453316</td>
<td>0.021194</td>
<td>0.024973</td>
<td>0.003548</td>
</tr>
</tbody>
</table>

Table S9: Energies for Cacodylic acid [Hartrees].

<table>
<thead>
<tr>
<th>Method</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>-2466.935873</td>
<td>0.088684</td>
<td>0.097943</td>
<td>0.056207</td>
<td>-2466.948013</td>
<td>0.088605</td>
<td>0.097867</td>
<td>0.056165</td>
</tr>
<tr>
<td>BLYP</td>
<td>-2466.090562</td>
<td>0.279969</td>
<td>0.297887</td>
<td>0.236482</td>
<td>-2466.113028</td>
<td>0.279548</td>
<td>0.297606</td>
<td>0.235946</td>
</tr>
<tr>
<td>B1LYP</td>
<td>-2466.676721</td>
<td>0.091543</td>
<td>0.100562</td>
<td>0.059397</td>
<td>-2466.689855</td>
<td>0.091407</td>
<td>0.100468</td>
<td>0.059192</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-2466.816236</td>
<td>0.091045</td>
<td>0.100113</td>
<td>0.058824</td>
<td>-2466.829297</td>
<td>0.090938</td>
<td>0.10026</td>
<td>0.058698</td>
</tr>
</tbody>
</table>

Table S10: Energies for (7R,8S,9R,10S)-BPT (tetrol) [Hartrees].

<table>
<thead>
<tr>
<th>Method</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
<th>$E^{KS}$</th>
<th>$Z$</th>
<th>$H_{corr}$</th>
<th>$G_{corr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>-1072.800177</td>
<td>0.308548</td>
<td>0.328628</td>
<td>0.262703</td>
<td>-1072.824353</td>
<td>0.307444</td>
<td>0.327839</td>
<td>0.261185</td>
</tr>
<tr>
<td>BLYP</td>
<td>-1072.545171</td>
<td>0.306560</td>
<td>0.326671</td>
<td>0.260714</td>
<td>-1072.573262</td>
<td>0.305650</td>
<td>0.326044</td>
<td>0.259498</td>
</tr>
<tr>
<td>B1LYP</td>
<td>-1072.406913</td>
<td>0.319189</td>
<td>0.338586</td>
<td>0.274015</td>
<td>-1072.431223</td>
<td>0.318186</td>
<td>0.337566</td>
<td>0.272631</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-1072.927368</td>
<td>0.317418</td>
<td>0.336907</td>
<td>0.272164</td>
<td>-1072.951644</td>
<td>0.316410</td>
<td>0.336178</td>
<td>0.270764</td>
</tr>
<tr>
<td></td>
<td>E&lt;sub&gt;KS&lt;/sub&gt;</td>
<td>Z</td>
<td>Hcorr</td>
<td>Gcorr</td>
<td>E&lt;sub&gt;KS&lt;/sub&gt;</td>
<td>Z</td>
<td>Hcorr</td>
<td>Gcorr</td>
</tr>
<tr>
<td>-----</td>
<td>-----------------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-----------------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td><strong>TS1</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BPW91</td>
<td>-1072.704756</td>
<td>0.302550</td>
<td>0.323642</td>
<td>0.255085</td>
<td>-1072.742406</td>
<td>0.302020</td>
<td>0.323584</td>
<td>0.253484</td>
</tr>
<tr>
<td>BLYP</td>
<td>-1072.458345</td>
<td>0.301620</td>
<td>0.322416</td>
<td>0.254886</td>
<td>-1072.503892</td>
<td>0.300159</td>
<td>0.321766</td>
<td>0.252128</td>
</tr>
<tr>
<td>B1LYP</td>
<td>-1072.304272</td>
<td>0.313686</td>
<td>0.333734</td>
<td>0.267854</td>
<td>-1072.346009</td>
<td>0.312646</td>
<td>0.333532</td>
<td>0.264712</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-1072.825945</td>
<td>0.312073</td>
<td>0.332147</td>
<td>0.266216</td>
<td>-1072.867183</td>
<td>0.310855</td>
<td>0.331831</td>
<td>0.262866</td>
</tr>
<tr>
<td><strong>TS2</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BPW91</td>
<td>-1072.735803</td>
<td>0.302844</td>
<td>0.322736</td>
<td>0.257132</td>
<td>-1072.760460</td>
<td>0.301437</td>
<td>0.321574</td>
<td>0.255135</td>
</tr>
<tr>
<td>BLYP</td>
<td>-1072.485746</td>
<td>0.300455</td>
<td>0.320370</td>
<td>0.254631</td>
<td>-1072.518721</td>
<td>0.297999</td>
<td>0.318575</td>
<td>0.250948</td>
</tr>
<tr>
<td>B1LYP</td>
<td>-1072.329565</td>
<td>0.313485</td>
<td>0.332753</td>
<td>0.267931</td>
<td>-1072.359592</td>
<td>0.312646</td>
<td>0.333532</td>
<td>0.264712</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-1072.852325</td>
<td>0.311690</td>
<td>0.331023</td>
<td>0.266234</td>
<td>-1072.882220</td>
<td>0.310287</td>
<td>0.329808</td>
<td>0.264420</td>
</tr>
<tr>
<td><strong>TS3</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BPW91</td>
<td>-3463.261806</td>
<td>0.367683</td>
<td>0.394851</td>
<td>0.311078</td>
<td>-3463.287157</td>
<td>0.366351</td>
<td>0.393984</td>
<td>0.309007</td>
</tr>
<tr>
<td>BLYP</td>
<td>-3462.834697</td>
<td>0.365210</td>
<td>0.392753</td>
<td>0.307809</td>
<td>-3462.869274</td>
<td>0.364025</td>
<td>0.391870</td>
<td>0.306263</td>
</tr>
<tr>
<td>B1LYP</td>
<td>-3462.620479</td>
<td>0.379336</td>
<td>0.406040</td>
<td>0.322785</td>
<td>-3462.651061</td>
<td>0.378173</td>
<td>0.405146</td>
<td>0.320742</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-3463.251015</td>
<td>0.377400</td>
<td>0.404180</td>
<td>0.320889</td>
<td>-3463.281408</td>
<td>0.376212</td>
<td>0.403270</td>
<td>0.318983</td>
</tr>
</tbody>
</table>
Table S12: Mulliken and NBO charges for (+)-anti-BPDE, TS1 (Triol), and (7R,8S,9R,10S)-BPT (Tetrol).

<table>
<thead>
<tr>
<th></th>
<th>Mulliken</th>
<th>NBO</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>6-31g*</td>
<td>6-31+g*</td>
</tr>
<tr>
<td>B1LYP</td>
<td>BPDE</td>
<td>Tetrol</td>
</tr>
<tr>
<td>C9</td>
<td>-0.07</td>
<td>-0.11</td>
</tr>
<tr>
<td>C9,H</td>
<td>+0.17</td>
<td>+0.13</td>
</tr>
<tr>
<td>C10</td>
<td>-0.23</td>
<td>-0.10</td>
</tr>
<tr>
<td>C10,H</td>
<td>+0.02</td>
<td>+0.15</td>
</tr>
<tr>
<td>O3</td>
<td>-0.33</td>
<td>-0.61</td>
</tr>
<tr>
<td>O4,H</td>
<td>NA</td>
<td>-0.63</td>
</tr>
<tr>
<td>Total</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>B3LYP</td>
<td>BPDE</td>
<td>Tetrol</td>
</tr>
<tr>
<td>C9</td>
<td>-0.07</td>
<td>-0.12</td>
</tr>
<tr>
<td>C9,H</td>
<td>+0.17</td>
<td>+0.12</td>
</tr>
<tr>
<td>C10</td>
<td>-0.23</td>
<td>-0.11</td>
</tr>
<tr>
<td>C10,H</td>
<td>+0.02</td>
<td>+0.14</td>
</tr>
<tr>
<td>O3</td>
<td>-0.33</td>
<td>-0.60</td>
</tr>
<tr>
<td>O4,H</td>
<td>NA</td>
<td>-0.61</td>
</tr>
<tr>
<td>Total</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

Table S13: Mulliken and NBO charges for (+)-anti-BPDE, TS2, and (7R,8S,9R,10S)-BPT (Tetrol).

<table>
<thead>
<tr>
<th></th>
<th>Mulliken</th>
<th>NBO</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>6-31g*</td>
<td>6-31+g*</td>
</tr>
<tr>
<td>B1LYP</td>
<td>BPDE</td>
<td>Tetrol</td>
</tr>
<tr>
<td>C9</td>
<td>-0.07</td>
<td>+0.03</td>
</tr>
<tr>
<td>C9,H</td>
<td>+0.17</td>
<td>+0.26</td>
</tr>
<tr>
<td>C10</td>
<td>-0.23</td>
<td>-0.30</td>
</tr>
<tr>
<td>C10,H</td>
<td>+0.02</td>
<td>+0.14</td>
</tr>
<tr>
<td>O3</td>
<td>-0.33</td>
<td>-0.67</td>
</tr>
<tr>
<td>H+</td>
<td>NA</td>
<td>+0.43</td>
</tr>
<tr>
<td>H2O</td>
<td>NA</td>
<td>+0.01</td>
</tr>
<tr>
<td>Total</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>B3LYP</td>
<td>BPDE</td>
<td>Tetrol</td>
</tr>
<tr>
<td>C9</td>
<td>-0.07</td>
<td>+0.02</td>
</tr>
<tr>
<td>C9,H</td>
<td>+0.17</td>
<td>+0.19</td>
</tr>
<tr>
<td>C10</td>
<td>-0.23</td>
<td>-0.31</td>
</tr>
<tr>
<td>C10,H</td>
<td>+0.02</td>
<td>+0.05</td>
</tr>
<tr>
<td>O3</td>
<td>-0.33</td>
<td>-0.66</td>
</tr>
<tr>
<td>H+</td>
<td>NA</td>
<td>+0.43</td>
</tr>
<tr>
<td>H2O</td>
<td>NA</td>
<td>+0.01</td>
</tr>
<tr>
<td>Total</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Table S14: Mulliken and NBO charges for (+)-anti-BPDE , TS3, and (7R,8S,9R,10S)-BPT (Tetrol).

<table>
<thead>
<tr>
<th></th>
<th>6-311g* Mulliken</th>
<th>6-311g* NBO</th>
<th>6-31+g* Mulliken</th>
<th>6-31+g* NBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>B3LYP</td>
<td>BPDE Transition</td>
<td>Tetrol</td>
<td>BPDE Transition</td>
<td>Tetrol</td>
</tr>
<tr>
<td>C9</td>
<td>-0.07</td>
<td>-0.09</td>
<td>+0.04</td>
<td>+0.09</td>
</tr>
<tr>
<td>C9,H</td>
<td>+0.17</td>
<td>+0.13</td>
<td>+0.26</td>
<td>+0.29</td>
</tr>
<tr>
<td>C10</td>
<td>-0.23</td>
<td>-0.17</td>
<td>-0.10</td>
<td>+0.09</td>
</tr>
<tr>
<td>C10,H</td>
<td>+0.02</td>
<td>+0.15</td>
<td>+0.14</td>
<td>+0.29</td>
</tr>
<tr>
<td>O3</td>
<td>-0.33</td>
<td>-0.57</td>
<td>-0.62</td>
<td>-0.57</td>
</tr>
<tr>
<td>H+</td>
<td>NA</td>
<td>+0.44</td>
<td>NA</td>
<td>+0.49</td>
</tr>
<tr>
<td>O4</td>
<td>NA</td>
<td>-0.82</td>
<td>NA</td>
<td>-1.13</td>
</tr>
<tr>
<td>As</td>
<td>NA</td>
<td>+1.23</td>
<td>NA</td>
<td>+2.09</td>
</tr>
<tr>
<td>Total</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>6-31+g* Mulliken</th>
<th>6-31+g* NBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>B3LYP</td>
<td>BPDE Transition</td>
<td>Tetrol</td>
</tr>
<tr>
<td>C9</td>
<td>-0.07</td>
<td>-0.10</td>
</tr>
<tr>
<td>C9,H</td>
<td>+0.17</td>
<td>+0.12</td>
</tr>
<tr>
<td>C10</td>
<td>-0.23</td>
<td>-0.17</td>
</tr>
<tr>
<td>C10,H</td>
<td>+0.02</td>
<td>+0.14</td>
</tr>
<tr>
<td>O3</td>
<td>-0.33</td>
<td>-0.56</td>
</tr>
<tr>
<td>H+</td>
<td>NA</td>
<td>+0.43</td>
</tr>
<tr>
<td>O4</td>
<td>NA</td>
<td>-0.81</td>
</tr>
<tr>
<td>As</td>
<td>NA</td>
<td>+1.20</td>
</tr>
<tr>
<td>Total</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Structural information. Angles $\phi_1 - 4$ are the dihedrals that the hydroxyl groups make with respect to the six membered ring to which they are attached. Dihedral angles are reported in the range -180 to 180. Hydroxyl are numbered starting at the bottom in counterclockwise order. The atoms involved in the dihedral angles ($\phi$) are given below. Fig. S1 displays relevant atom labels.

$$
\begin{align*}
\phi_1 & : C'' - C' - C7 - O1 \\
\phi_2 & : C' - C7 - C8 - O2 \\
\phi_3 & : C'' - C10 - C9 - O3 \\
\phi_4 & : C' - C''' - C10 - O4
\end{align*}
$$

Figure S1: Scheme illustrating labeling convention. Note that only the tetrol has a bound O4 oxygen. For the transition structures, O4 refers to the oxygen that donates a proton to BPDE (either from a water molecule or cacodylic acid). O4 is not present in BPDE by itself.

Table S15: Selected TS1 geometric parameters. Distances given in Å and angles in degrees.

<table>
<thead>
<tr>
<th>Method</th>
<th>$\phi_1$</th>
<th>$\phi_2$</th>
<th>$\phi_3$</th>
<th>$\phi_4$</th>
<th>C9-C10</th>
<th>C10-O3</th>
<th>C9-O3</th>
<th>C10-O4</th>
<th>O4-C10-C9</th>
<th>C10-O4-H</th>
</tr>
</thead>
<tbody>
<tr>
<td>6-311g*</td>
<td>-162.769</td>
<td>-101.589</td>
<td>170.284</td>
<td>1.503</td>
<td>2.407</td>
<td>1.459</td>
<td>2.773</td>
<td>110.278</td>
<td>146.493</td>
<td></td>
</tr>
<tr>
<td>BLYP</td>
<td>-162.398</td>
<td>179.502</td>
<td>-93.784</td>
<td>1.509</td>
<td>2.429</td>
<td>1.472</td>
<td>2.992</td>
<td>114.644</td>
<td>82.827</td>
<td></td>
</tr>
<tr>
<td>B1LYP</td>
<td>164.868</td>
<td>179.603</td>
<td>-98.630</td>
<td>-161.442</td>
<td>1.502</td>
<td>2.376</td>
<td>1.441</td>
<td>2.843</td>
<td>111.667</td>
<td>95.816</td>
</tr>
<tr>
<td>B3LYP</td>
<td>-164.529</td>
<td>179.709</td>
<td>-96.572</td>
<td>-164.047</td>
<td>1.502</td>
<td>2.385</td>
<td>1.443</td>
<td>2.867</td>
<td>112.677</td>
<td>92.988</td>
</tr>
<tr>
<td>6-311+g*</td>
<td>-161.897</td>
<td>-99.477</td>
<td>175.319</td>
<td>1.504</td>
<td>2.409</td>
<td>1.458</td>
<td>2.937</td>
<td>112.519</td>
<td>150.233</td>
<td></td>
</tr>
<tr>
<td>BLYP</td>
<td>-162.674</td>
<td>179.600</td>
<td>-93.004</td>
<td>-161.538</td>
<td>1.508</td>
<td>2.428</td>
<td>1.471</td>
<td>2.928</td>
<td>110.457</td>
<td>117.551</td>
</tr>
</tbody>
</table>
Table S16: Selected TS2 geometric parameters. Distances given in Å and angles in degrees.

<table>
<thead>
<tr>
<th>Method</th>
<th>C9-C10</th>
<th>C10-O3</th>
<th>C9-O3</th>
<th>O4-C10-C9</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>2.354</td>
<td>1.384</td>
<td>2.354</td>
<td>92.690</td>
</tr>
<tr>
<td>BLYP</td>
<td>2.384</td>
<td>1.394</td>
<td>2.295</td>
<td>92.926</td>
</tr>
<tr>
<td>B1LYP</td>
<td>2.371</td>
<td>1.374</td>
<td>2.281</td>
<td>93.289</td>
</tr>
<tr>
<td>B3LYP</td>
<td>2.365</td>
<td>1.376</td>
<td>2.294</td>
<td>93.160</td>
</tr>
</tbody>
</table>

Table S17: Selected TS3 geometric parameters. Distances given in Å and angles in degrees.

<table>
<thead>
<tr>
<th>Method</th>
<th>C9-C10</th>
<th>C10-O3</th>
<th>C9-O3</th>
<th>O4-C10-C9</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>2.381</td>
<td>1.382</td>
<td>2.322</td>
<td>93.304</td>
</tr>
<tr>
<td>BLYP</td>
<td>2.384</td>
<td>1.394</td>
<td>2.295</td>
<td>92.926</td>
</tr>
<tr>
<td>B1LYP</td>
<td>2.408</td>
<td>1.383</td>
<td>2.215</td>
<td>94.030</td>
</tr>
<tr>
<td>B3LYP</td>
<td>2.398</td>
<td>1.384</td>
<td>2.240</td>
<td>94.014</td>
</tr>
</tbody>
</table>

Table S18: Selected (+)-anti-BPDE geometric parameters. Distances given in Å and angles in degrees.

<table>
<thead>
<tr>
<th>Method</th>
<th>C9-C10</th>
<th>C10-O3</th>
<th>C9-O3</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>2.226</td>
<td>1.427</td>
<td>3.592</td>
</tr>
<tr>
<td>BLYP</td>
<td>2.141</td>
<td>1.435</td>
<td>3.586</td>
</tr>
<tr>
<td>B1LYP</td>
<td>2.087</td>
<td>1.412</td>
<td>3.542</td>
</tr>
<tr>
<td>B3LYP</td>
<td>2.087</td>
<td>1.412</td>
<td>3.537</td>
</tr>
</tbody>
</table>

Table S19: Selected (7R,8S,9R,10S)-BPT (Tetrol) geometric parameters. Distances given in Å and angles in degrees.

<table>
<thead>
<tr>
<th>Method</th>
<th>C9-C10</th>
<th>C10-O3</th>
<th>C9-O3</th>
</tr>
</thead>
<tbody>
<tr>
<td>BPW91</td>
<td>2.410</td>
<td>1.437</td>
<td>1.452</td>
</tr>
<tr>
<td>BLYP</td>
<td>2.421</td>
<td>1.435</td>
<td>1.451</td>
</tr>
<tr>
<td>B1LYP</td>
<td>2.435</td>
<td>1.446</td>
<td>1.461</td>
</tr>
<tr>
<td>B3LYP</td>
<td>2.435</td>
<td>1.446</td>
<td>1.461</td>
</tr>
</tbody>
</table>
Table S20: As-C10 distances for hydrogen bonded (HB...BPDE) and TS3 structures.

<table>
<thead>
<tr>
<th></th>
<th>6-311g*</th>
<th></th>
<th></th>
<th>6-311+g*</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HB...BPDE</td>
<td>TS3</td>
<td>HB...BPDE</td>
<td>TS3</td>
</tr>
<tr>
<td>BPW91</td>
<td>3.985</td>
<td>3.877</td>
<td>4.071</td>
<td>3.954</td>
</tr>
<tr>
<td>BLYP</td>
<td>4.018</td>
<td>3.918</td>
<td>4.128</td>
<td>4.026</td>
</tr>
<tr>
<td>B1LYP</td>
<td>3.991</td>
<td>3.884</td>
<td>4.073</td>
<td>3.977</td>
</tr>
<tr>
<td>B3LYP</td>
<td>4.005</td>
<td>3.879</td>
<td>4.071</td>
<td>3.968</td>
</tr>
</tbody>
</table>
Table S21: BPW91 6-311g* TS1 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.916179</td>
<td>0.807790</td>
<td>0.125517</td>
</tr>
<tr>
<td>C</td>
<td>-0.921177</td>
<td>1.716607</td>
<td>-0.152883</td>
</tr>
<tr>
<td>C</td>
<td>0.439217</td>
<td>1.277392</td>
<td>-0.403596</td>
</tr>
<tr>
<td>C</td>
<td>0.721059</td>
<td>-0.157246</td>
<td>-0.421019</td>
</tr>
<tr>
<td>C</td>
<td>2.029027</td>
<td>-0.666781</td>
<td>-0.670956</td>
</tr>
<tr>
<td>C</td>
<td>2.262788</td>
<td>-2.027226</td>
<td>-0.676767</td>
</tr>
<tr>
<td>C</td>
<td>1.222765</td>
<td>-2.972686</td>
<td>-0.425532</td>
</tr>
<tr>
<td>C</td>
<td>1.448664</td>
<td>-4.370483</td>
<td>-0.427361</td>
</tr>
<tr>
<td>C</td>
<td>0.409506</td>
<td>-5.263612</td>
<td>-0.160255</td>
</tr>
<tr>
<td>C</td>
<td>-0.877636</td>
<td>-4.788220</td>
<td>0.115002</td>
</tr>
<tr>
<td>C</td>
<td>-1.149738</td>
<td>-3.402567</td>
<td>0.128042</td>
</tr>
<tr>
<td>C</td>
<td>-2.454284</td>
<td>-2.886436</td>
<td>0.409228</td>
</tr>
<tr>
<td>C</td>
<td>-2.698602</td>
<td>-1.530505</td>
<td>0.415702</td>
</tr>
<tr>
<td>C</td>
<td>-1.660474</td>
<td>-0.592952</td>
<td>0.142545</td>
</tr>
<tr>
<td>C</td>
<td>-0.337481</td>
<td>-1.074681</td>
<td>-0.142449</td>
</tr>
<tr>
<td>C</td>
<td>-0.089577</td>
<td>-2.480265</td>
<td>-0.147675</td>
</tr>
<tr>
<td>C</td>
<td>1.456378</td>
<td>2.206292</td>
<td>-0.593047</td>
</tr>
<tr>
<td>C</td>
<td>1.236520</td>
<td>3.685830</td>
<td>-0.444312</td>
</tr>
<tr>
<td>C</td>
<td>-0.060958</td>
<td>4.033011</td>
<td>0.283669</td>
</tr>
<tr>
<td>C</td>
<td>-1.218441</td>
<td>3.187656</td>
<td>-0.281784</td>
</tr>
<tr>
<td>O</td>
<td>1.113360</td>
<td>4.276642</td>
<td>-1.772314</td>
</tr>
<tr>
<td>O</td>
<td>-0.367615</td>
<td>5.423558</td>
<td>0.174942</td>
</tr>
<tr>
<td>O</td>
<td>-2.445890</td>
<td>3.521196</td>
<td>0.359264</td>
</tr>
<tr>
<td>H</td>
<td>-2.928642</td>
<td>1.165502</td>
<td>0.316098</td>
</tr>
<tr>
<td>H</td>
<td>2.864882</td>
<td>0.032618</td>
<td>-0.840627</td>
</tr>
<tr>
<td>H</td>
<td>3.271867</td>
<td>-2.399801</td>
<td>-0.871016</td>
</tr>
<tr>
<td>H</td>
<td>2.451884</td>
<td>-4.746078</td>
<td>-0.639848</td>
</tr>
<tr>
<td>H</td>
<td>0.600975</td>
<td>-6.337810</td>
<td>-0.165579</td>
</tr>
<tr>
<td>H</td>
<td>-1.687280</td>
<td>-5.491217</td>
<td>0.322495</td>
</tr>
<tr>
<td>H</td>
<td>-3.263060</td>
<td>-3.588910</td>
<td>0.621632</td>
</tr>
<tr>
<td>H</td>
<td>-3.701173</td>
<td>-1.155476</td>
<td>0.630930</td>
</tr>
<tr>
<td>H</td>
<td>2.497083</td>
<td>1.896858</td>
<td>-0.816020</td>
</tr>
<tr>
<td>H</td>
<td>2.095643</td>
<td>4.139815</td>
<td>0.075025</td>
</tr>
<tr>
<td>H</td>
<td>0.041115</td>
<td>3.813731</td>
<td>1.357178</td>
</tr>
<tr>
<td>H</td>
<td>-1.286360</td>
<td>3.417010</td>
<td>-1.365781</td>
</tr>
<tr>
<td>H</td>
<td>-0.113940</td>
<td>5.670399</td>
<td>-0.738111</td>
</tr>
<tr>
<td>H</td>
<td>-2.477516</td>
<td>4.496809</td>
<td>0.346407</td>
</tr>
<tr>
<td>H</td>
<td>4.883090</td>
<td>1.028846</td>
<td>-0.45933</td>
</tr>
<tr>
<td>O</td>
<td>4.169444</td>
<td>1.644588</td>
<td>-0.707940</td>
</tr>
<tr>
<td>H</td>
<td>2.009735</td>
<td>4.401714</td>
<td>-2.128387</td>
</tr>
</tbody>
</table>
Table S22: BPW91 6-311+g* TS1 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.919964</td>
<td>0.810197</td>
<td>0.118197</td>
</tr>
<tr>
<td>C</td>
<td>-0.927194</td>
<td>1.719413</td>
<td>-0.155458</td>
</tr>
<tr>
<td>C</td>
<td>0.439511</td>
<td>1.279244</td>
<td>-0.392963</td>
</tr>
<tr>
<td>C</td>
<td>0.721507</td>
<td>-0.160493</td>
<td>-0.412174</td>
</tr>
<tr>
<td>C</td>
<td>2.024925</td>
<td>-0.671404</td>
<td>-0.662852</td>
</tr>
<tr>
<td>C</td>
<td>2.257408</td>
<td>-2.034509</td>
<td>-0.666191</td>
</tr>
<tr>
<td>C</td>
<td>1.216545</td>
<td>-2.976322</td>
<td>-0.416200</td>
</tr>
<tr>
<td>C</td>
<td>1.440485</td>
<td>-4.375659</td>
<td>-0.416487</td>
</tr>
<tr>
<td>C</td>
<td>0.398925</td>
<td>-5.267436</td>
<td>-0.154540</td>
</tr>
<tr>
<td>C</td>
<td>-0.888649</td>
<td>-4.788349</td>
<td>0.114283</td>
</tr>
<tr>
<td>C</td>
<td>-1.157503</td>
<td>-3.401287</td>
<td>0.125148</td>
</tr>
<tr>
<td>C</td>
<td>-2.461437</td>
<td>-2.884087</td>
<td>0.399567</td>
</tr>
<tr>
<td>C</td>
<td>-2.704253</td>
<td>-1.525981</td>
<td>0.404516</td>
</tr>
<tr>
<td>C</td>
<td>-1.662977</td>
<td>-0.593015</td>
<td>0.137012</td>
</tr>
<tr>
<td>C</td>
<td>-0.339953</td>
<td>-1.076278</td>
<td>-0.140402</td>
</tr>
<tr>
<td>C</td>
<td>-0.095039</td>
<td>-2.481518</td>
<td>-0.145076</td>
</tr>
<tr>
<td>C</td>
<td>1.454321</td>
<td>2.206806</td>
<td>-0.557450</td>
</tr>
<tr>
<td>C</td>
<td>1.227078</td>
<td>3.689490</td>
<td>-0.443321</td>
</tr>
<tr>
<td>C</td>
<td>-0.071128</td>
<td>4.039252</td>
<td>0.285506</td>
</tr>
<tr>
<td>C</td>
<td>-1.229773</td>
<td>3.191230</td>
<td>-0.275015</td>
</tr>
<tr>
<td>O</td>
<td>1.104435</td>
<td>4.250618</td>
<td>-1.783084</td>
</tr>
<tr>
<td>O</td>
<td>-0.373456</td>
<td>5.431305</td>
<td>0.182038</td>
</tr>
<tr>
<td>O</td>
<td>-2.459940</td>
<td>3.505029</td>
<td>0.376820</td>
</tr>
<tr>
<td>H</td>
<td>-2.934603</td>
<td>1.163394</td>
<td>0.304406</td>
</tr>
<tr>
<td>H</td>
<td>2.867935</td>
<td>0.017605</td>
<td>-0.834436</td>
</tr>
<tr>
<td>H</td>
<td>3.266515</td>
<td>-2.406877</td>
<td>-0.806796</td>
</tr>
<tr>
<td>H</td>
<td>2.444194</td>
<td>-4.752750</td>
<td>-0.624337</td>
</tr>
<tr>
<td>H</td>
<td>0.588276</td>
<td>-6.341961</td>
<td>-0.158633</td>
</tr>
<tr>
<td>H</td>
<td>-1.700994</td>
<td>-5.489370</td>
<td>0.318351</td>
</tr>
<tr>
<td>H</td>
<td>-3.273014</td>
<td>-3.584694</td>
<td>0.607726</td>
</tr>
<tr>
<td>H</td>
<td>-3.707528</td>
<td>-1.149890</td>
<td>0.614066</td>
</tr>
<tr>
<td>H</td>
<td>2.498302</td>
<td>1.900419</td>
<td>-0.743867</td>
</tr>
<tr>
<td>H</td>
<td>2.081621</td>
<td>4.160360</td>
<td>0.067109</td>
</tr>
<tr>
<td>H</td>
<td>0.039194</td>
<td>3.824118</td>
<td>1.358707</td>
</tr>
<tr>
<td>H</td>
<td>-1.317245</td>
<td>3.424714</td>
<td>-1.355774</td>
</tr>
<tr>
<td>H</td>
<td>-0.149609</td>
<td>5.693761</td>
<td>-0.734643</td>
</tr>
<tr>
<td>H</td>
<td>-2.533997</td>
<td>4.478395</td>
<td>0.355455</td>
</tr>
<tr>
<td>H</td>
<td>5.113450</td>
<td>1.130862</td>
<td>-0.490362</td>
</tr>
<tr>
<td>O</td>
<td>4.295419</td>
<td>1.523052</td>
<td>-0.849107</td>
</tr>
<tr>
<td>H</td>
<td>1.997190</td>
<td>4.433528</td>
<td>-2.125256</td>
</tr>
</tbody>
</table>
Table S23: BLYP 6-311g* TS1 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.894233</td>
<td>0.818028</td>
<td>0.112894</td>
</tr>
<tr>
<td>C</td>
<td>-0.909677</td>
<td>1.726567</td>
<td>-0.168176</td>
</tr>
<tr>
<td>C</td>
<td>0.479365</td>
<td>1.288224</td>
<td>-0.381624</td>
</tr>
<tr>
<td>C</td>
<td>0.752348</td>
<td>-0.161993</td>
<td>-0.432437</td>
</tr>
<tr>
<td>C</td>
<td>2.045634</td>
<td>-0.688310</td>
<td>-0.731664</td>
</tr>
<tr>
<td>C</td>
<td>2.267654</td>
<td>-2.055108</td>
<td>-0.751371</td>
</tr>
<tr>
<td>C</td>
<td>1.232503</td>
<td>-2.994477</td>
<td>-0.452224</td>
</tr>
<tr>
<td>C</td>
<td>1.449120</td>
<td>-4.398697</td>
<td>-0.449671</td>
</tr>
<tr>
<td>C</td>
<td>0.406682</td>
<td>-5.285853</td>
<td>-0.165483</td>
</tr>
<tr>
<td>C</td>
<td>-0.878440</td>
<td>-4.799333</td>
<td>0.126549</td>
</tr>
<tr>
<td>C</td>
<td>-1.141620</td>
<td>-3.408049</td>
<td>0.133979</td>
</tr>
<tr>
<td>C</td>
<td>-2.442271</td>
<td>-2.881944</td>
<td>0.428551</td>
</tr>
<tr>
<td>C</td>
<td>-2.679435</td>
<td>-1.520706</td>
<td>0.432059</td>
</tr>
<tr>
<td>C</td>
<td>-1.639355</td>
<td>-0.588947</td>
<td>0.137757</td>
</tr>
<tr>
<td>C</td>
<td>-0.317395</td>
<td>-1.077954</td>
<td>-0.163660</td>
</tr>
<tr>
<td>C</td>
<td>-0.076673</td>
<td>-2.489723</td>
<td>-0.161352</td>
</tr>
<tr>
<td>C</td>
<td>1.503561</td>
<td>2.220721</td>
<td>-0.446852</td>
</tr>
<tr>
<td>C</td>
<td>1.258296</td>
<td>3.708213</td>
<td>-0.386040</td>
</tr>
<tr>
<td>C</td>
<td>-0.069102</td>
<td>4.066328</td>
<td>0.298949</td>
</tr>
<tr>
<td>C</td>
<td>-1.208504</td>
<td>3.202771</td>
<td>-0.297811</td>
</tr>
<tr>
<td>O</td>
<td>1.148663</td>
<td>4.236588</td>
<td>-1.755213</td>
</tr>
<tr>
<td>O</td>
<td>-0.372195</td>
<td>5.463092</td>
<td>0.156981</td>
</tr>
<tr>
<td>O</td>
<td>-2.462866</td>
<td>3.519734</td>
<td>0.323102</td>
</tr>
<tr>
<td>H</td>
<td>-2.906831</td>
<td>1.174502</td>
<td>0.300553</td>
</tr>
<tr>
<td>H</td>
<td>2.885429</td>
<td>-0.012115</td>
<td>-0.958695</td>
</tr>
<tr>
<td>H</td>
<td>3.260979</td>
<td>-2.432620</td>
<td>-1.005737</td>
</tr>
<tr>
<td>H</td>
<td>2.447634</td>
<td>-4.781396</td>
<td>-0.673173</td>
</tr>
<tr>
<td>H</td>
<td>0.591225</td>
<td>-6.360944</td>
<td>-0.167760</td>
</tr>
<tr>
<td>H</td>
<td>-1.686098</td>
<td>-5.496063</td>
<td>0.352344</td>
</tr>
<tr>
<td>H</td>
<td>-3.253015</td>
<td>-3.578194</td>
<td>0.651840</td>
</tr>
<tr>
<td>H</td>
<td>-3.677040</td>
<td>-1.139685</td>
<td>0.657493</td>
</tr>
<tr>
<td>H</td>
<td>2.560117</td>
<td>1.931556</td>
<td>-0.658722</td>
</tr>
<tr>
<td>H</td>
<td>2.095159</td>
<td>4.213447</td>
<td>0.120040</td>
</tr>
<tr>
<td>H</td>
<td>-0.005476</td>
<td>3.869949</td>
<td>1.378845</td>
</tr>
<tr>
<td>H</td>
<td>-1.260171</td>
<td>3.437353</td>
<td>-1.379737</td>
</tr>
<tr>
<td>H</td>
<td>-0.115657</td>
<td>5.693246</td>
<td>-0.762085</td>
</tr>
<tr>
<td>H</td>
<td>-2.525106</td>
<td>4.495211</td>
<td>0.288874</td>
</tr>
<tr>
<td>H</td>
<td>4.307432</td>
<td>1.130402</td>
<td>-0.087066</td>
</tr>
<tr>
<td>O</td>
<td>4.336878</td>
<td>1.445700</td>
<td>-1.015015</td>
</tr>
<tr>
<td>H</td>
<td>2.049654</td>
<td>4.421387</td>
<td>-2.078566</td>
</tr>
</tbody>
</table>
Table S24: BLYP 6-311+g* TS1 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.919832</td>
<td>0.802064</td>
<td>0.046401</td>
</tr>
<tr>
<td>C</td>
<td>-0.905889</td>
<td>1.705245</td>
<td>-0.184056</td>
</tr>
<tr>
<td>C</td>
<td>0.478345</td>
<td>1.251741</td>
<td>-0.299296</td>
</tr>
<tr>
<td>C</td>
<td>0.743311</td>
<td>-0.194585</td>
<td>-0.347016</td>
</tr>
<tr>
<td>C</td>
<td>2.041118</td>
<td>-0.722014</td>
<td>-0.620370</td>
</tr>
<tr>
<td>C</td>
<td>2.261430</td>
<td>-2.089854</td>
<td>-0.631595</td>
</tr>
<tr>
<td>C</td>
<td>1.210480</td>
<td>-3.024500</td>
<td>-0.370904</td>
</tr>
<tr>
<td>C</td>
<td>1.421074</td>
<td>-4.429924</td>
<td>-0.365517</td>
</tr>
<tr>
<td>C</td>
<td>0.364651</td>
<td>-5.312917</td>
<td>-0.115411</td>
</tr>
<tr>
<td>C</td>
<td>-0.926982</td>
<td>-4.821121</td>
<td>0.129915</td>
</tr>
<tr>
<td>C</td>
<td>-1.185843</td>
<td>-3.428512</td>
<td>0.129533</td>
</tr>
<tr>
<td>C</td>
<td>-2.496350</td>
<td>-2.895398</td>
<td>0.365786</td>
</tr>
<tr>
<td>C</td>
<td>-2.729920</td>
<td>-1.533078</td>
<td>0.349584</td>
</tr>
<tr>
<td>C</td>
<td>-1.671757</td>
<td>-0.605656</td>
<td>0.105286</td>
</tr>
<tr>
<td>C</td>
<td>-0.338575</td>
<td>-1.103959</td>
<td>-0.119330</td>
</tr>
<tr>
<td>C</td>
<td>-0.105365</td>
<td>-2.515966</td>
<td>-0.119345</td>
</tr>
<tr>
<td>C</td>
<td>1.520999</td>
<td>2.166346</td>
<td>-0.243182</td>
</tr>
<tr>
<td>C</td>
<td>1.296874</td>
<td>3.657526</td>
<td>-0.198943</td>
</tr>
<tr>
<td>C</td>
<td>-0.083758</td>
<td>4.033864</td>
<td>0.362669</td>
</tr>
<tr>
<td>C</td>
<td>-1.185877</td>
<td>3.187523</td>
<td>-0.327261</td>
</tr>
<tr>
<td>O</td>
<td>1.331424</td>
<td>4.192062</td>
<td>1.568952</td>
</tr>
<tr>
<td>O</td>
<td>-0.351903</td>
<td>5.440041</td>
<td>0.214256</td>
</tr>
<tr>
<td>O</td>
<td>-2.486639</td>
<td>3.505484</td>
<td>0.201781</td>
</tr>
<tr>
<td>H</td>
<td>-2.940478</td>
<td>1.161303</td>
<td>0.173927</td>
</tr>
<tr>
<td>H</td>
<td>2.867724</td>
<td>-0.045325</td>
<td>-0.851104</td>
</tr>
<tr>
<td>H</td>
<td>3.261108</td>
<td>-2.471282</td>
<td>-0.851519</td>
</tr>
<tr>
<td>H</td>
<td>2.422795</td>
<td>-4.817856</td>
<td>-0.560349</td>
</tr>
<tr>
<td>H</td>
<td>0.544462</td>
<td>-6.388777</td>
<td>-0.113001</td>
</tr>
<tr>
<td>H</td>
<td>-1.747493</td>
<td>-5.515167</td>
<td>0.322481</td>
</tr>
<tr>
<td>H</td>
<td>-3.319246</td>
<td>-3.587564</td>
<td>0.554837</td>
</tr>
<tr>
<td>H</td>
<td>-3.737016</td>
<td>-1.149040</td>
<td>0.520930</td>
</tr>
<tr>
<td>H</td>
<td>2.575598</td>
<td>1.859329</td>
<td>-0.294204</td>
</tr>
<tr>
<td>H</td>
<td>2.089294</td>
<td>4.146703</td>
<td>0.387595</td>
</tr>
<tr>
<td>H</td>
<td>-0.108854</td>
<td>3.834606</td>
<td>1.443423</td>
</tr>
<tr>
<td>H</td>
<td>-1.166036</td>
<td>3.403336</td>
<td>-1.407105</td>
</tr>
<tr>
<td>H</td>
<td>-0.028144</td>
<td>5.701927</td>
<td>-0.674163</td>
</tr>
<tr>
<td>H</td>
<td>-2.581732</td>
<td>4.476930</td>
<td>0.135198</td>
</tr>
<tr>
<td>H</td>
<td>4.684643</td>
<td>2.266603</td>
<td>1.712813</td>
</tr>
<tr>
<td>O</td>
<td>4.213395</td>
<td>1.563298</td>
<td>-1.221105</td>
</tr>
<tr>
<td>H</td>
<td>2.258845</td>
<td>4.180475</td>
<td>-1.876583</td>
</tr>
</tbody>
</table>
Table S25: B1LYP 6-311g* TS1 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.903434</td>
<td>0.812822</td>
<td>0.085528</td>
</tr>
<tr>
<td>C</td>
<td>-0.912386</td>
<td>1.710165</td>
<td>-0.176268</td>
</tr>
<tr>
<td>C</td>
<td>0.460416</td>
<td>1.267158</td>
<td>-0.346615</td>
</tr>
<tr>
<td>C</td>
<td>0.737785</td>
<td>-0.166816</td>
<td>-0.406615</td>
</tr>
<tr>
<td>C</td>
<td>2.027448</td>
<td>-0.676132</td>
<td>-0.715913</td>
</tr>
<tr>
<td>C</td>
<td>2.247042</td>
<td>-2.030950</td>
<td>-0.728343</td>
</tr>
<tr>
<td>C</td>
<td>1.217638</td>
<td>-2.968009</td>
<td>-0.428548</td>
</tr>
<tr>
<td>C</td>
<td>1.437156</td>
<td>-4.359514</td>
<td>-0.425105</td>
</tr>
<tr>
<td>C</td>
<td>0.405045</td>
<td>-5.243841</td>
<td>-0.136486</td>
</tr>
<tr>
<td>C</td>
<td>-0.870512</td>
<td>-4.763484</td>
<td>0.150892</td>
</tr>
<tr>
<td>C</td>
<td>-1.134760</td>
<td>-3.384020</td>
<td>0.153845</td>
</tr>
<tr>
<td>C</td>
<td>-2.431768</td>
<td>-2.860632</td>
<td>0.434583</td>
</tr>
<tr>
<td>C</td>
<td>-2.673965</td>
<td>-1.512913</td>
<td>0.422926</td>
</tr>
<tr>
<td>C</td>
<td>-1.637589</td>
<td>-0.585265</td>
<td>0.137164</td>
</tr>
<tr>
<td>C</td>
<td>-0.321937</td>
<td>-1.072577</td>
<td>-0.135581</td>
</tr>
<tr>
<td>C</td>
<td>-0.080537</td>
<td>-2.473606</td>
<td>-0.136049</td>
</tr>
<tr>
<td>C</td>
<td>1.486526</td>
<td>2.176567</td>
<td>-0.344649</td>
</tr>
<tr>
<td>C</td>
<td>1.265959</td>
<td>3.658008</td>
<td>-0.238079</td>
</tr>
<tr>
<td>C</td>
<td>-0.104035</td>
<td>4.028635</td>
<td>0.317012</td>
</tr>
<tr>
<td>C</td>
<td>-1.196691</td>
<td>3.179337</td>
<td>-0.344666</td>
</tr>
<tr>
<td>O</td>
<td>1.331304</td>
<td>4.206511</td>
<td>-1.568723</td>
</tr>
<tr>
<td>O</td>
<td>-0.380752</td>
<td>5.408860</td>
<td>0.142224</td>
</tr>
<tr>
<td>O</td>
<td>-2.470277</td>
<td>3.502604</td>
<td>0.180744</td>
</tr>
<tr>
<td>H</td>
<td>-2.915884</td>
<td>1.161098</td>
<td>0.238403</td>
</tr>
<tr>
<td>H</td>
<td>2.836985</td>
<td>0.014787</td>
<td>-0.983638</td>
</tr>
<tr>
<td>H</td>
<td>3.233050</td>
<td>2.408026</td>
<td>-0.977989</td>
</tr>
<tr>
<td>H</td>
<td>2.427001</td>
<td>4.738004</td>
<td>-0.651962</td>
</tr>
<tr>
<td>H</td>
<td>0.591786</td>
<td>-6.310275</td>
<td>-0.136596</td>
</tr>
<tr>
<td>H</td>
<td>-1.673185</td>
<td>-5.456741</td>
<td>0.373715</td>
</tr>
<tr>
<td>H</td>
<td>-3.236118</td>
<td>-3.552775</td>
<td>0.655044</td>
</tr>
<tr>
<td>H</td>
<td>-3.668283</td>
<td>-1.136479</td>
<td>0.629599</td>
</tr>
<tr>
<td>H</td>
<td>2.540536</td>
<td>1.887474</td>
<td>-0.567168</td>
</tr>
<tr>
<td>H</td>
<td>2.051303</td>
<td>4.109026</td>
<td>0.375497</td>
</tr>
<tr>
<td>H</td>
<td>-0.127316</td>
<td>3.840523</td>
<td>1.392496</td>
</tr>
<tr>
<td>H</td>
<td>-1.173050</td>
<td>3.391861</td>
<td>-1.423279</td>
</tr>
<tr>
<td>H</td>
<td>-0.044671</td>
<td>5.654619</td>
<td>-0.730648</td>
</tr>
<tr>
<td>H</td>
<td>-2.545880</td>
<td>4.463353</td>
<td>0.132860</td>
</tr>
<tr>
<td>H</td>
<td>4.481151</td>
<td>1.424001</td>
<td>-0.557933</td>
</tr>
<tr>
<td>O</td>
<td>4.051349</td>
<td>1.571172</td>
<td>-1.412519</td>
</tr>
<tr>
<td>H</td>
<td>2.242534</td>
<td>4.143788</td>
<td>-1.878683</td>
</tr>
</tbody>
</table>
Table S26: B1LYP 6-311+g* TS1 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.92684</td>
<td>0.799917</td>
<td>0.066966</td>
</tr>
<tr>
<td>C</td>
<td>-0.929046</td>
<td>1.695197</td>
<td>-0.168340</td>
</tr>
<tr>
<td>C</td>
<td>0.446011</td>
<td>1.245200</td>
<td>-0.312246</td>
</tr>
<tr>
<td>C</td>
<td>0.720656</td>
<td>-0.190677</td>
<td>-0.369564</td>
</tr>
<tr>
<td>C</td>
<td>2.011502</td>
<td>-0.706299</td>
<td>-0.648928</td>
</tr>
<tr>
<td>C</td>
<td>2.232536</td>
<td>-2.062242</td>
<td>-0.659821</td>
</tr>
<tr>
<td>C</td>
<td>1.191701</td>
<td>-2.994001</td>
<td>-0.391866</td>
</tr>
<tr>
<td>C</td>
<td>1.406124</td>
<td>-4.387544</td>
<td>-0.390054</td>
</tr>
<tr>
<td>C</td>
<td>0.364708</td>
<td>-5.268644</td>
<td>-0.125780</td>
</tr>
<tr>
<td>C</td>
<td>-0.914809</td>
<td>-4.783000</td>
<td>0.137377</td>
</tr>
<tr>
<td>C</td>
<td>-1.173288</td>
<td>-3.401782</td>
<td>0.140563</td>
</tr>
<tr>
<td>C</td>
<td>-2.472983</td>
<td>-2.874971</td>
<td>0.396388</td>
</tr>
<tr>
<td>C</td>
<td>-2.710436</td>
<td>-1.524428</td>
<td>0.382986</td>
</tr>
<tr>
<td>C</td>
<td>-1.665310</td>
<td>-0.601693</td>
<td>0.123069</td>
</tr>
<tr>
<td>C</td>
<td>-0.345439</td>
<td>-1.093493</td>
<td>-0.120542</td>
</tr>
<tr>
<td>C</td>
<td>-0.109651</td>
<td>-2.494951</td>
<td>-0.123791</td>
</tr>
<tr>
<td>C</td>
<td>1.469827</td>
<td>2.149574</td>
<td>-0.312380</td>
</tr>
<tr>
<td>C</td>
<td>1.270970</td>
<td>3.631944</td>
<td>-0.189846</td>
</tr>
<tr>
<td>C</td>
<td>-0.111383</td>
<td>4.012420</td>
<td>0.331667</td>
</tr>
<tr>
<td>C</td>
<td>-1.200884</td>
<td>3.166520</td>
<td>-0.343523</td>
</tr>
<tr>
<td>O</td>
<td>1.406107</td>
<td>4.207613</td>
<td>-1.502533</td>
</tr>
<tr>
<td>O</td>
<td>-0.375621</td>
<td>5.396876</td>
<td>0.157780</td>
</tr>
<tr>
<td>O</td>
<td>-2.484442</td>
<td>3.401943</td>
<td>0.163698</td>
</tr>
<tr>
<td>H</td>
<td>-2.942885</td>
<td>1.146876</td>
<td>0.195661</td>
</tr>
<tr>
<td>H</td>
<td>2.832941</td>
<td>-0.031534</td>
<td>-0.869862</td>
</tr>
<tr>
<td>H</td>
<td>3.225038</td>
<td>-2.438821</td>
<td>-0.880642</td>
</tr>
<tr>
<td>H</td>
<td>2.398799</td>
<td>-4.769272</td>
<td>-0.598261</td>
</tr>
<tr>
<td>H</td>
<td>0.546581</td>
<td>-6.335857</td>
<td>-0.126282</td>
</tr>
<tr>
<td>H</td>
<td>-1.724936</td>
<td>-5.473605</td>
<td>0.340731</td>
</tr>
<tr>
<td>H</td>
<td>-3.284586</td>
<td>-3.564225</td>
<td>0.598598</td>
</tr>
<tr>
<td>H</td>
<td>-3.707965</td>
<td>-1.145859</td>
<td>0.568952</td>
</tr>
<tr>
<td>H</td>
<td>2.515840</td>
<td>1.865146</td>
<td>-0.457068</td>
</tr>
<tr>
<td>H</td>
<td>2.040743</td>
<td>4.049826</td>
<td>0.465357</td>
</tr>
<tr>
<td>H</td>
<td>-0.150054</td>
<td>3.827202</td>
<td>1.407007</td>
</tr>
<tr>
<td>H</td>
<td>-1.170630</td>
<td>3.377073</td>
<td>-1.422107</td>
</tr>
<tr>
<td>H</td>
<td>-0.023027</td>
<td>5.664165</td>
<td>-0.702574</td>
</tr>
<tr>
<td>H</td>
<td>-2.588592</td>
<td>4.448984</td>
<td>0.090043</td>
</tr>
<tr>
<td>H</td>
<td>5.053819</td>
<td>2.056969</td>
<td>-1.369428</td>
</tr>
<tr>
<td>O</td>
<td>4.137789</td>
<td>1.761098</td>
<td>-1.298820</td>
</tr>
<tr>
<td>H</td>
<td>2.309941</td>
<td>4.059264</td>
<td>-1.812106</td>
</tr>
</tbody>
</table>
Table S27: B3LYP 6-311g* TS1 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.898136</td>
<td>0.814702</td>
<td>0.087722</td>
</tr>
<tr>
<td>C</td>
<td>-0.907922</td>
<td>1.712619</td>
<td>-0.182318</td>
</tr>
<tr>
<td>C</td>
<td>0.465103</td>
<td>1.270825</td>
<td>-0.357789</td>
</tr>
<tr>
<td>C</td>
<td>0.740397</td>
<td>-0.164532</td>
<td>-0.414053</td>
</tr>
<tr>
<td>C</td>
<td>2.028099</td>
<td>-0.675957</td>
<td>-0.724887</td>
</tr>
<tr>
<td>C</td>
<td>2.247615</td>
<td>-2.031895</td>
<td>-0.738453</td>
</tr>
<tr>
<td>C</td>
<td>1.218992</td>
<td>-2.967961</td>
<td>-0.435866</td>
</tr>
<tr>
<td>C</td>
<td>1.437834</td>
<td>-4.360367</td>
<td>-0.432185</td>
</tr>
<tr>
<td>C</td>
<td>-0.869291</td>
<td>-4.762660</td>
<td>0.150134</td>
</tr>
<tr>
<td>C</td>
<td>-1.133304</td>
<td>-3.382457</td>
<td>0.153097</td>
</tr>
<tr>
<td>C</td>
<td>-2.429007</td>
<td>-2.858967</td>
<td>0.438394</td>
</tr>
<tr>
<td>C</td>
<td>-2.670343</td>
<td>-1.510127</td>
<td>0.427805</td>
</tr>
<tr>
<td>C</td>
<td>-1.634793</td>
<td>-0.583161</td>
<td>0.137346</td>
</tr>
<tr>
<td>C</td>
<td>-0.319855</td>
<td>-1.070669</td>
<td>-0.141207</td>
</tr>
<tr>
<td>C</td>
<td>-0.078975</td>
<td>-2.471967</td>
<td>-0.140812</td>
</tr>
<tr>
<td>C</td>
<td>1.491142</td>
<td>2.183589</td>
<td>-0.356144</td>
</tr>
<tr>
<td>C</td>
<td>1.261911</td>
<td>3.665212</td>
<td>-0.265863</td>
</tr>
<tr>
<td>C</td>
<td>-0.099398</td>
<td>4.029156</td>
<td>0.315135</td>
</tr>
<tr>
<td>C</td>
<td>-1.197139</td>
<td>3.179487</td>
<td>-0.341183</td>
</tr>
<tr>
<td>O</td>
<td>1.285511</td>
<td>4.205436</td>
<td>-1.603747</td>
</tr>
<tr>
<td>O</td>
<td>-0.381090</td>
<td>5.410100</td>
<td>0.152150</td>
</tr>
<tr>
<td>O</td>
<td>-2.467512</td>
<td>3.501359</td>
<td>0.195640</td>
</tr>
<tr>
<td>H</td>
<td>-2.909616</td>
<td>1.165773</td>
<td>0.249188</td>
</tr>
<tr>
<td>H</td>
<td>2.841654</td>
<td>0.014180</td>
<td>-0.090367</td>
</tr>
<tr>
<td>H</td>
<td>3.233950</td>
<td>2.409430</td>
<td>-0.991323</td>
</tr>
<tr>
<td>H</td>
<td>2.428161</td>
<td>4.739602</td>
<td>-0.661188</td>
</tr>
<tr>
<td>H</td>
<td>0.591834</td>
<td>6.311761</td>
<td>-0.140770</td>
</tr>
<tr>
<td>H</td>
<td>-1.672535</td>
<td>-5.455993</td>
<td>0.376248</td>
</tr>
<tr>
<td>H</td>
<td>-3.233627</td>
<td>-3.551548</td>
<td>0.662098</td>
</tr>
<tr>
<td>H</td>
<td>-3.664618</td>
<td>-1.132641</td>
<td>0.639022</td>
</tr>
<tr>
<td>H</td>
<td>2.548763</td>
<td>1.891669</td>
<td>-0.559108</td>
</tr>
<tr>
<td>H</td>
<td>2.056672</td>
<td>4.132762</td>
<td>0.324230</td>
</tr>
<tr>
<td>H</td>
<td>-0.107564</td>
<td>3.833277</td>
<td>1.390561</td>
</tr>
<tr>
<td>H</td>
<td>-1.181196</td>
<td>3.399911</td>
<td>-1.419981</td>
</tr>
<tr>
<td>H</td>
<td>-0.061415</td>
<td>5.655976</td>
<td>-0.729281</td>
</tr>
<tr>
<td>H</td>
<td>-2.537134</td>
<td>4.465028</td>
<td>0.160426</td>
</tr>
<tr>
<td>H</td>
<td>4.439604</td>
<td>1.319730</td>
<td>-0.461928</td>
</tr>
<tr>
<td>O</td>
<td>4.100665</td>
<td>1.527076</td>
<td>-1.346316</td>
</tr>
<tr>
<td>H</td>
<td>2.199948</td>
<td>4.218508</td>
<td>-1.913180</td>
</tr>
</tbody>
</table>
Table S28: B3LYP 6-311+g* **TS1** coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.91932</td>
<td>0.802064</td>
<td>0.046401</td>
</tr>
<tr>
<td>C</td>
<td>-0.90589</td>
<td>1.705245</td>
<td>-0.184056</td>
</tr>
<tr>
<td>C</td>
<td>0.478345</td>
<td>1.251741</td>
<td>-0.299296</td>
</tr>
<tr>
<td>C</td>
<td>0.743311</td>
<td>-0.194585</td>
<td>-0.347016</td>
</tr>
<tr>
<td>C</td>
<td>2.041118</td>
<td>-0.722014</td>
<td>-0.620370</td>
</tr>
<tr>
<td>C</td>
<td>2.261430</td>
<td>-2.089854</td>
<td>-0.631595</td>
</tr>
<tr>
<td>C</td>
<td>1.210480</td>
<td>-3.024500</td>
<td>-0.370904</td>
</tr>
<tr>
<td>C</td>
<td>1.421074</td>
<td>-4.429924</td>
<td>-0.365517</td>
</tr>
<tr>
<td>C</td>
<td>0.364651</td>
<td>-5.312917</td>
<td>-0.115411</td>
</tr>
<tr>
<td>C</td>
<td>-0.926982</td>
<td>-4.821121</td>
<td>0.129915</td>
</tr>
<tr>
<td>C</td>
<td>-1.185843</td>
<td>-3.428512</td>
<td>0.129533</td>
</tr>
<tr>
<td>C</td>
<td>-2.496350</td>
<td>-2.895398</td>
<td>0.365786</td>
</tr>
<tr>
<td>C</td>
<td>-2.729920</td>
<td>-1.533078</td>
<td>0.349584</td>
</tr>
<tr>
<td>C</td>
<td>-1.671757</td>
<td>-0.605656</td>
<td>0.105286</td>
</tr>
<tr>
<td>C</td>
<td>-0.338575</td>
<td>-1.103959</td>
<td>-0.119330</td>
</tr>
<tr>
<td>C</td>
<td>-0.105365</td>
<td>-2.515966</td>
<td>-0.119345</td>
</tr>
<tr>
<td>C</td>
<td>1.520099</td>
<td>2.166346</td>
<td>-0.243182</td>
</tr>
<tr>
<td>C</td>
<td>1.296874</td>
<td>3.657526</td>
<td>-0.198943</td>
</tr>
<tr>
<td>C</td>
<td>-0.083758</td>
<td>4.033864</td>
<td>0.362669</td>
</tr>
<tr>
<td>C</td>
<td>-1.185877</td>
<td>3.187523</td>
<td>-0.327261</td>
</tr>
<tr>
<td>O</td>
<td>1.331424</td>
<td>4.192062</td>
<td>-1.568952</td>
</tr>
<tr>
<td>O</td>
<td>-0.351903</td>
<td>5.440041</td>
<td>0.214256</td>
</tr>
<tr>
<td>O</td>
<td>-2.486639</td>
<td>3.505484</td>
<td>0.201781</td>
</tr>
<tr>
<td>H</td>
<td>-2.940478</td>
<td>1.161303</td>
<td>0.173927</td>
</tr>
<tr>
<td>H</td>
<td>2.867724</td>
<td>-0.045325</td>
<td>-0.851104</td>
</tr>
<tr>
<td>H</td>
<td>3.261108</td>
<td>-2.471282</td>
<td>-0.851519</td>
</tr>
<tr>
<td>H</td>
<td>2.422795</td>
<td>-4.817856</td>
<td>-0.560349</td>
</tr>
<tr>
<td>H</td>
<td>0.544462</td>
<td>-6.388777</td>
<td>-0.113001</td>
</tr>
<tr>
<td>H</td>
<td>-1.747493</td>
<td>-5.515167</td>
<td>0.322481</td>
</tr>
<tr>
<td>H</td>
<td>-3.319246</td>
<td>-3.587564</td>
<td>0.554837</td>
</tr>
<tr>
<td>H</td>
<td>-3.737016</td>
<td>-1.149040</td>
<td>0.520930</td>
</tr>
<tr>
<td>H</td>
<td>2.575598</td>
<td>1.859329</td>
<td>-0.294204</td>
</tr>
<tr>
<td>H</td>
<td>2.089294</td>
<td>4.146703</td>
<td>0.387595</td>
</tr>
<tr>
<td>H</td>
<td>-0.108854</td>
<td>3.834606</td>
<td>1.443423</td>
</tr>
<tr>
<td>H</td>
<td>-1.160036</td>
<td>3.430336</td>
<td>-1.407105</td>
</tr>
<tr>
<td>H</td>
<td>-0.028144</td>
<td>5.701927</td>
<td>-0.674163</td>
</tr>
<tr>
<td>H</td>
<td>-2.581732</td>
<td>4.476930</td>
<td>0.135198</td>
</tr>
<tr>
<td>H</td>
<td>4.684643</td>
<td>2.266603</td>
<td>-1.712813</td>
</tr>
<tr>
<td>O</td>
<td>4.213395</td>
<td>1.563298</td>
<td>-1.221105</td>
</tr>
<tr>
<td>H</td>
<td>2.258845</td>
<td>4.180475</td>
<td>-1.876583</td>
</tr>
</tbody>
</table>
Table S29: BPW91 6-311g* TS2 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.850850</td>
<td>0.819911</td>
<td>-0.178353</td>
</tr>
<tr>
<td>C</td>
<td>-0.808219</td>
<td>1.719524</td>
<td>-0.340533</td>
</tr>
<tr>
<td>C</td>
<td>0.557066</td>
<td>1.253229</td>
<td>-0.351394</td>
</tr>
<tr>
<td>C</td>
<td>0.813071</td>
<td>-0.171591</td>
<td>-0.313041</td>
</tr>
<tr>
<td>C</td>
<td>2.126795</td>
<td>-0.713300</td>
<td>-0.456472</td>
</tr>
<tr>
<td>C</td>
<td>2.353352</td>
<td>-2.069413</td>
<td>-0.392696</td>
</tr>
<tr>
<td>C</td>
<td>1.283584</td>
<td>-2.955998</td>
<td>-0.189233</td>
</tr>
<tr>
<td>C</td>
<td>1.492311</td>
<td>-4.392962</td>
<td>-0.110773</td>
</tr>
<tr>
<td>C</td>
<td>0.418226</td>
<td>-5.265348</td>
<td>0.071602</td>
</tr>
<tr>
<td>C</td>
<td>-0.888002</td>
<td>-4.770998</td>
<td>0.173824</td>
</tr>
<tr>
<td>C</td>
<td>-1.144903</td>
<td>-3.386611</td>
<td>0.096930</td>
</tr>
<tr>
<td>C</td>
<td>-2.471932</td>
<td>-2.848189</td>
<td>0.189161</td>
</tr>
<tr>
<td>C</td>
<td>-2.701011</td>
<td>-1.496889</td>
<td>0.104233</td>
</tr>
<tr>
<td>C</td>
<td>-1.623012</td>
<td>-0.571904</td>
<td>-0.072502</td>
</tr>
<tr>
<td>C</td>
<td>-0.280132</td>
<td>-1.075872</td>
<td>-0.153888</td>
</tr>
<tr>
<td>C</td>
<td>-0.047575</td>
<td>-2.482882</td>
<td>-0.082043</td>
</tr>
<tr>
<td>C</td>
<td>1.603185</td>
<td>2.190222</td>
<td>-0.217215</td>
</tr>
<tr>
<td>C</td>
<td>1.358391</td>
<td>3.680427</td>
<td>-0.365152</td>
</tr>
<tr>
<td>C</td>
<td>-0.004607</td>
<td>3.983291</td>
<td>0.334873</td>
</tr>
<tr>
<td>C</td>
<td>-1.076567</td>
<td>3.191136</td>
<td>-0.434778</td>
</tr>
<tr>
<td>O</td>
<td>1.310719</td>
<td>3.981891</td>
<td>-1.715508</td>
</tr>
<tr>
<td>O</td>
<td>-0.365396</td>
<td>5.363216</td>
<td>0.227774</td>
</tr>
<tr>
<td>O</td>
<td>-2.390367</td>
<td>3.510255</td>
<td>0.017381</td>
</tr>
<tr>
<td>H</td>
<td>-2.871129</td>
<td>1.199668</td>
<td>-0.118506</td>
</tr>
<tr>
<td>H</td>
<td>2.954716</td>
<td>-0.038827</td>
<td>-0.660586</td>
</tr>
<tr>
<td>H</td>
<td>3.368379</td>
<td>-2.456071</td>
<td>-0.510161</td>
</tr>
<tr>
<td>H</td>
<td>2.508382</td>
<td>-4.784469</td>
<td>-0.195584</td>
</tr>
<tr>
<td>H</td>
<td>0.596318</td>
<td>-6.340436</td>
<td>0.132296</td>
</tr>
<tr>
<td>H</td>
<td>-1.723363</td>
<td>-5.460610</td>
<td>0.314078</td>
</tr>
<tr>
<td>H</td>
<td>-3.308078</td>
<td>-3.537896</td>
<td>0.325241</td>
</tr>
<tr>
<td>H</td>
<td>-3.718912</td>
<td>-1.106796</td>
<td>0.169833</td>
</tr>
<tr>
<td>H</td>
<td>2.551805</td>
<td>1.845945</td>
<td>0.193075</td>
</tr>
<tr>
<td>H</td>
<td>2.144292</td>
<td>4.252414</td>
<td>0.178752</td>
</tr>
<tr>
<td>H</td>
<td>0.008698</td>
<td>3.668409</td>
<td>1.392865</td>
</tr>
<tr>
<td>H</td>
<td>-0.937551</td>
<td>3.498848</td>
<td>-1.492740</td>
</tr>
<tr>
<td>H</td>
<td>-0.118864</td>
<td>5.807250</td>
<td>1.055246</td>
</tr>
<tr>
<td>H</td>
<td>-2.392041</td>
<td>4.484430</td>
<td>0.080643</td>
</tr>
<tr>
<td>H</td>
<td>3.740299</td>
<td>2.386226</td>
<td>-1.926418</td>
</tr>
<tr>
<td>O</td>
<td>2.857192</td>
<td>2.086273</td>
<td>-2.206334</td>
</tr>
<tr>
<td>H</td>
<td>2.244710</td>
<td>2.955407</td>
<td>-2.194417</td>
</tr>
</tbody>
</table>
Table S30: BPW91 6-311+g* TS2 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.839368</td>
<td>0.822207</td>
<td>-0.204988</td>
</tr>
<tr>
<td>C</td>
<td>-0.795638</td>
<td>1.721694</td>
<td>-0.345010</td>
</tr>
<tr>
<td>C</td>
<td>0.570581</td>
<td>1.255839</td>
<td>-0.348034</td>
</tr>
<tr>
<td>C</td>
<td>0.828776</td>
<td>-0.171273</td>
<td>-0.294326</td>
</tr>
<tr>
<td>C</td>
<td>2.144113</td>
<td>-0.717038</td>
<td>-0.392306</td>
</tr>
<tr>
<td>C</td>
<td>2.367566</td>
<td>-2.073977</td>
<td>-0.316746</td>
</tr>
<tr>
<td>C</td>
<td>1.291395</td>
<td>-2.998670</td>
<td>-0.147698</td>
</tr>
<tr>
<td>C</td>
<td>1.497001</td>
<td>-4.396032</td>
<td>-0.059994</td>
</tr>
<tr>
<td>C</td>
<td>0.417421</td>
<td>-5.267241</td>
<td>0.095615</td>
</tr>
<tr>
<td>C</td>
<td>-0.890294</td>
<td>-4.769996</td>
<td>0.162138</td>
</tr>
<tr>
<td>C</td>
<td>-1.142625</td>
<td>-3.384895</td>
<td>0.075483</td>
</tr>
<tr>
<td>C</td>
<td>-2.470481</td>
<td>-2.845997</td>
<td>0.135074</td>
</tr>
<tr>
<td>C</td>
<td>-2.695417</td>
<td>-1.493381</td>
<td>0.046111</td>
</tr>
<tr>
<td>C</td>
<td>-1.612068</td>
<td>-0.571528</td>
<td>-0.105317</td>
</tr>
<tr>
<td>C</td>
<td>-0.268273</td>
<td>-1.075550</td>
<td>-0.158347</td>
</tr>
<tr>
<td>C</td>
<td>-0.040333</td>
<td>-2.482922</td>
<td>-0.077456</td>
</tr>
<tr>
<td>C</td>
<td>1.617886</td>
<td>2.190914</td>
<td>-0.253068</td>
</tr>
<tr>
<td>C</td>
<td>1.377375</td>
<td>3.692916</td>
<td>-0.346535</td>
</tr>
<tr>
<td>C</td>
<td>0.012801</td>
<td>3.975158</td>
<td>0.352308</td>
</tr>
<tr>
<td>C</td>
<td>-1.065377</td>
<td>3.198175</td>
<td>-0.420830</td>
</tr>
<tr>
<td>O</td>
<td>1.362178</td>
<td>4.075835</td>
<td>-1.684893</td>
</tr>
<tr>
<td>O</td>
<td>-0.346774</td>
<td>5.369010</td>
<td>0.291149</td>
</tr>
<tr>
<td>O</td>
<td>-2.380822</td>
<td>3.499484</td>
<td>0.054000</td>
</tr>
<tr>
<td>H</td>
<td>-2.861865</td>
<td>1.197553</td>
<td>-0.157556</td>
</tr>
<tr>
<td>H</td>
<td>2.990212</td>
<td>-0.051616</td>
<td>-0.558845</td>
</tr>
<tr>
<td>H</td>
<td>3.386437</td>
<td>-2.460462</td>
<td>-0.390016</td>
</tr>
<tr>
<td>H</td>
<td>2.514813</td>
<td>-4.788625</td>
<td>-0.115624</td>
</tr>
<tr>
<td>H</td>
<td>0.592281</td>
<td>-6.342482</td>
<td>0.163829</td>
</tr>
<tr>
<td>H</td>
<td>-1.730399</td>
<td>-5.457848</td>
<td>0.282362</td>
</tr>
<tr>
<td>H</td>
<td>-3.310931</td>
<td>-3.534246</td>
<td>0.251577</td>
</tr>
<tr>
<td>H</td>
<td>-3.713895</td>
<td>-1.101616</td>
<td>0.089818</td>
</tr>
<tr>
<td>H</td>
<td>2.586555</td>
<td>1.848436</td>
<td>0.109031</td>
</tr>
<tr>
<td>H</td>
<td>2.162905</td>
<td>4.223744</td>
<td>0.235519</td>
</tr>
<tr>
<td>H</td>
<td>0.035498</td>
<td>3.639540</td>
<td>1.403531</td>
</tr>
<tr>
<td>H</td>
<td>-0.962061</td>
<td>3.519679</td>
<td>-1.476790</td>
</tr>
<tr>
<td>H</td>
<td>-0.091009</td>
<td>5.788170</td>
<td>1.125825</td>
</tr>
<tr>
<td>H</td>
<td>-2.410840</td>
<td>4.473496</td>
<td>0.120480</td>
</tr>
<tr>
<td>H</td>
<td>3.620406</td>
<td>2.272597</td>
<td>-2.197078</td>
</tr>
<tr>
<td>O</td>
<td>2.671886</td>
<td>2.093995</td>
<td>-2.331026</td>
</tr>
<tr>
<td>H</td>
<td>2.149066</td>
<td>3.045963</td>
<td>-2.234889</td>
</tr>
</tbody>
</table>
Table S31: BLYP 6-311g* TS2 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.84480</td>
<td>0.827764</td>
<td>-0.158115</td>
</tr>
<tr>
<td>C</td>
<td>-0.797228</td>
<td>1.725559</td>
<td>-0.323693</td>
</tr>
<tr>
<td>C</td>
<td>0.569923</td>
<td>1.252603</td>
<td>-0.353748</td>
</tr>
<tr>
<td>C</td>
<td>0.820874</td>
<td>-0.178380</td>
<td>-0.321521</td>
</tr>
<tr>
<td>C</td>
<td>2.134275</td>
<td>-0.731981</td>
<td>-0.476411</td>
</tr>
<tr>
<td>C</td>
<td>2.353212</td>
<td>-2.092058</td>
<td>-0.419035</td>
</tr>
<tr>
<td>C</td>
<td>1.277277</td>
<td>-3.017264</td>
<td>-0.211222</td>
</tr>
<tr>
<td>C</td>
<td>1.478268</td>
<td>-4.419260</td>
<td>-0.138821</td>
</tr>
<tr>
<td>C</td>
<td>0.397850</td>
<td>-5.288008</td>
<td>0.049383</td>
</tr>
<tr>
<td>C</td>
<td>-0.907820</td>
<td>-4.785573</td>
<td>0.163722</td>
</tr>
<tr>
<td>C</td>
<td>-1.158979</td>
<td>-3.396068</td>
<td>0.093303</td>
</tr>
<tr>
<td>C</td>
<td>-2.485927</td>
<td>-2.847878</td>
<td>0.198088</td>
</tr>
<tr>
<td>C</td>
<td>-2.708045</td>
<td>-1.492633</td>
<td>0.120013</td>
</tr>
<tr>
<td>C</td>
<td>-1.623390</td>
<td>-0.569431</td>
<td>-0.062059</td>
</tr>
<tr>
<td>C</td>
<td>-0.279669</td>
<td>-1.081285</td>
<td>-0.156958</td>
</tr>
<tr>
<td>C</td>
<td>-0.054177</td>
<td>-2.494688</td>
<td>-0.091607</td>
</tr>
<tr>
<td>C</td>
<td>1.628479</td>
<td>2.188828</td>
<td>-0.246327</td>
</tr>
<tr>
<td>C</td>
<td>1.388890</td>
<td>3.696112</td>
<td>-0.369608</td>
</tr>
<tr>
<td>C</td>
<td>0.027738</td>
<td>3.997528</td>
<td>0.349079</td>
</tr>
<tr>
<td>C</td>
<td>-1.065520</td>
<td>3.208815</td>
<td>-0.401431</td>
</tr>
<tr>
<td>O</td>
<td>1.335412</td>
<td>4.039977</td>
<td>-1.719160</td>
</tr>
<tr>
<td>O</td>
<td>-0.335015</td>
<td>5.390591</td>
<td>0.254737</td>
</tr>
<tr>
<td>O</td>
<td>-2.377339</td>
<td>3.521921</td>
<td>0.101931</td>
</tr>
<tr>
<td>H</td>
<td>-2.861680</td>
<td>1.211407</td>
<td>-0.084917</td>
</tr>
<tr>
<td>H</td>
<td>2.960338</td>
<td>-0.065285</td>
<td>-0.690665</td>
</tr>
<tr>
<td>H</td>
<td>3.365300</td>
<td>-2.483503</td>
<td>-0.543895</td>
</tr>
<tr>
<td>H</td>
<td>2.490918</td>
<td>-4.816927</td>
<td>-0.232562</td>
</tr>
<tr>
<td>H</td>
<td>0.570219</td>
<td>-6.364122</td>
<td>0.105176</td>
</tr>
<tr>
<td>H</td>
<td>-1.745210</td>
<td>-5.471449</td>
<td>0.308337</td>
</tr>
<tr>
<td>H</td>
<td>-3.324878</td>
<td>-3.533010</td>
<td>0.338168</td>
</tr>
<tr>
<td>H</td>
<td>-3.722832</td>
<td>-1.096867</td>
<td>0.195556</td>
</tr>
<tr>
<td>H</td>
<td>2.574936</td>
<td>1.845223</td>
<td>0.166639</td>
</tr>
<tr>
<td>H</td>
<td>2.186395</td>
<td>4.245111</td>
<td>0.181408</td>
</tr>
<tr>
<td>H</td>
<td>0.055741</td>
<td>3.684457</td>
<td>1.406539</td>
</tr>
<tr>
<td>H</td>
<td>-0.975022</td>
<td>3.526712</td>
<td>-1.458591</td>
</tr>
<tr>
<td>H</td>
<td>-0.059024</td>
<td>5.835481</td>
<td>1.072974</td>
</tr>
<tr>
<td>H</td>
<td>-2.382262</td>
<td>4.497787</td>
<td>0.172340</td>
</tr>
<tr>
<td>H</td>
<td>3.682186</td>
<td>2.345008</td>
<td>-1.989559</td>
</tr>
<tr>
<td>O</td>
<td>2.771254</td>
<td>2.088861</td>
<td>-2.234425</td>
</tr>
<tr>
<td>H</td>
<td>2.194291</td>
<td>3.006833</td>
<td>-2.222583</td>
</tr>
</tbody>
</table>
Table S32: BLYP 6-311+g* TS2 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.835820</td>
<td>0.819849</td>
<td>-0.211883</td>
</tr>
<tr>
<td>C</td>
<td>-0.790107</td>
<td>1.720648</td>
<td>-0.337398</td>
</tr>
<tr>
<td>C</td>
<td>0.582766</td>
<td>1.254729</td>
<td>-0.334905</td>
</tr>
<tr>
<td>C</td>
<td>0.841812</td>
<td>-0.180121</td>
<td>-0.277776</td>
</tr>
<tr>
<td>C</td>
<td>2.160513</td>
<td>-0.732931</td>
<td>-0.358512</td>
</tr>
<tr>
<td>C</td>
<td>2.379825</td>
<td>-2.093639</td>
<td>-0.281233</td>
</tr>
<tr>
<td>C</td>
<td>1.297564</td>
<td>-3.019719</td>
<td>-0.126797</td>
</tr>
<tr>
<td>C</td>
<td>1.499074</td>
<td>-4.421678</td>
<td>-0.038106</td>
</tr>
<tr>
<td>C</td>
<td>0.413199</td>
<td>-5.292938</td>
<td>0.104358</td>
</tr>
<tr>
<td>C</td>
<td>-0.897304</td>
<td>-4.791716</td>
<td>0.156834</td>
</tr>
<tr>
<td>C</td>
<td>-1.147003</td>
<td>-3.402081</td>
<td>0.069153</td>
</tr>
<tr>
<td>C</td>
<td>-2.477635</td>
<td>-2.858494</td>
<td>0.114650</td>
</tr>
<tr>
<td>C</td>
<td>-2.699087</td>
<td>-1.501995</td>
<td>0.025194</td>
</tr>
<tr>
<td>C</td>
<td>-1.609952</td>
<td>-0.579430</td>
<td>-0.112935</td>
</tr>
<tr>
<td>C</td>
<td>-0.261970</td>
<td>-1.086219</td>
<td>-0.153016</td>
</tr>
<tr>
<td>C</td>
<td>-0.037555</td>
<td>-2.498969</td>
<td>-0.070610</td>
</tr>
<tr>
<td>C</td>
<td>1.633034</td>
<td>2.190541</td>
<td>-0.271909</td>
</tr>
<tr>
<td>C</td>
<td>1.399287</td>
<td>3.707494</td>
<td>-0.321543</td>
</tr>
<tr>
<td>C</td>
<td>0.019066</td>
<td>3.991667</td>
<td>0.352363</td>
</tr>
<tr>
<td>C</td>
<td>-1.063560</td>
<td>3.207649</td>
<td>-0.416087</td>
</tr>
<tr>
<td>O</td>
<td>1.428984</td>
<td>4.148813</td>
<td>-1.658805</td>
</tr>
<tr>
<td>O</td>
<td>-0.345392</td>
<td>5.389766</td>
<td>0.286138</td>
</tr>
<tr>
<td>O</td>
<td>-2.387728</td>
<td>3.501870</td>
<td>0.080426</td>
</tr>
<tr>
<td>H</td>
<td>-2.858733</td>
<td>1.192647</td>
<td>-0.174561</td>
</tr>
<tr>
<td>H</td>
<td>3.013746</td>
<td>-0.073839</td>
<td>-0.505973</td>
</tr>
<tr>
<td>H</td>
<td>3.398881</td>
<td>-2.481067</td>
<td>-0.346164</td>
</tr>
<tr>
<td>H</td>
<td>2.515964</td>
<td>-4.816846</td>
<td>-0.082326</td>
</tr>
<tr>
<td>H</td>
<td>0.584885</td>
<td>-6.368241</td>
<td>0.173082</td>
</tr>
<tr>
<td>H</td>
<td>-1.739428</td>
<td>-5.478153</td>
<td>0.266411</td>
</tr>
<tr>
<td>H</td>
<td>-3.320817</td>
<td>-3.544412</td>
<td>0.220468</td>
</tr>
<tr>
<td>H</td>
<td>-3.716829</td>
<td>-1.108592</td>
<td>0.058436</td>
</tr>
<tr>
<td>H</td>
<td>2.617473</td>
<td>1.850166</td>
<td>0.039811</td>
</tr>
<tr>
<td>H</td>
<td>2.181134</td>
<td>4.204594</td>
<td>0.291378</td>
</tr>
<tr>
<td>H</td>
<td>0.033905</td>
<td>3.667458</td>
<td>1.406222</td>
</tr>
<tr>
<td>H</td>
<td>-0.990735</td>
<td>3.526540</td>
<td>-1.472361</td>
</tr>
<tr>
<td>H</td>
<td>-0.064857</td>
<td>5.828567</td>
<td>1.110221</td>
</tr>
<tr>
<td>H</td>
<td>-2.432223</td>
<td>4.477961</td>
<td>0.140983</td>
</tr>
<tr>
<td>H</td>
<td>3.555880</td>
<td>2.248919</td>
<td>-2.319049</td>
</tr>
<tr>
<td>O</td>
<td>2.589245</td>
<td>2.143640</td>
<td>-2.419641</td>
</tr>
<tr>
<td>H</td>
<td>2.099541</td>
<td>3.168474</td>
<td>-2.234061</td>
</tr>
</tbody>
</table>
Table S33: BLYP 6-311g* TS2 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.835393</td>
<td>0.817059</td>
<td>-0.195811</td>
</tr>
<tr>
<td>C</td>
<td>-0.798008</td>
<td>1.712338</td>
<td>-0.334015</td>
</tr>
<tr>
<td>C</td>
<td>0.560053</td>
<td>1.247494</td>
<td>-0.339017</td>
</tr>
<tr>
<td>C</td>
<td>0.821045</td>
<td>-0.169345</td>
<td>-0.292400</td>
</tr>
<tr>
<td>C</td>
<td>2.136088</td>
<td>-0.711923</td>
<td>-0.405781</td>
</tr>
<tr>
<td>C</td>
<td>2.357087</td>
<td>-2.057703</td>
<td>-0.337858</td>
</tr>
<tr>
<td>C</td>
<td>1.285099</td>
<td>-2.983968</td>
<td>-0.161200</td>
</tr>
<tr>
<td>C</td>
<td>1.492168</td>
<td>-4.372799</td>
<td>-0.080561</td>
</tr>
<tr>
<td>C</td>
<td>0.419985</td>
<td>-5.241682</td>
<td>0.077452</td>
</tr>
<tr>
<td>C</td>
<td>-0.881608</td>
<td>-4.748550</td>
<td>0.152793</td>
</tr>
<tr>
<td>C</td>
<td>-1.133652</td>
<td>-3.371965</td>
<td>0.072853</td>
</tr>
<tr>
<td>C</td>
<td>-2.460038</td>
<td>-2.833198</td>
<td>0.140035</td>
</tr>
<tr>
<td>C</td>
<td>-2.685704</td>
<td>-1.492515</td>
<td>0.055709</td>
</tr>
<tr>
<td>C</td>
<td>-1.605119</td>
<td>-0.568926</td>
<td>-0.097865</td>
</tr>
<tr>
<td>C</td>
<td>-0.268709</td>
<td>-1.069907</td>
<td>-0.156864</td>
</tr>
<tr>
<td>C</td>
<td>-0.039207</td>
<td>-2.473740</td>
<td>-0.081833</td>
</tr>
<tr>
<td>C</td>
<td>1.602155</td>
<td>2.183467</td>
<td>-0.236935</td>
</tr>
<tr>
<td>C</td>
<td>1.358445</td>
<td>3.688025</td>
<td>-0.365871</td>
</tr>
<tr>
<td>C</td>
<td>0.002434</td>
<td>3.971648</td>
<td>0.331441</td>
</tr>
<tr>
<td>C</td>
<td>-1.075030</td>
<td>3.187874</td>
<td>-0.414712</td>
</tr>
<tr>
<td>O</td>
<td>1.335286</td>
<td>4.034582</td>
<td>-1.695270</td>
</tr>
<tr>
<td>O</td>
<td>-0.373311</td>
<td>5.342583</td>
<td>0.249349</td>
</tr>
<tr>
<td>O</td>
<td>-2.372092</td>
<td>3.478549</td>
<td>0.086705</td>
</tr>
<tr>
<td>H</td>
<td>-2.849288</td>
<td>1.189552</td>
<td>-0.144491</td>
</tr>
<tr>
<td>H</td>
<td>2.967606</td>
<td>-0.048509</td>
<td>-0.590992</td>
</tr>
<tr>
<td>H</td>
<td>3.366788</td>
<td>-2.441865</td>
<td>-0.429552</td>
</tr>
<tr>
<td>H</td>
<td>2.501997</td>
<td>-4.761545</td>
<td>-0.143559</td>
</tr>
<tr>
<td>H</td>
<td>0.595186</td>
<td>-6.308681</td>
<td>0.140154</td>
</tr>
<tr>
<td>H</td>
<td>-1.713225</td>
<td>-5.433047</td>
<td>0.274161</td>
</tr>
<tr>
<td>H</td>
<td>-3.292163</td>
<td>-3.518136</td>
<td>0.257247</td>
</tr>
<tr>
<td>H</td>
<td>-3.695858</td>
<td>-1.103454</td>
<td>0.103847</td>
</tr>
<tr>
<td>H</td>
<td>2.554347</td>
<td>1.848496</td>
<td>0.145907</td>
</tr>
<tr>
<td>H</td>
<td>2.145464</td>
<td>4.215629</td>
<td>0.206767</td>
</tr>
<tr>
<td>H</td>
<td>0.023255</td>
<td>3.653282</td>
<td>1.380704</td>
</tr>
<tr>
<td>H</td>
<td>-0.993939</td>
<td>3.497234</td>
<td>-1.464236</td>
</tr>
<tr>
<td>H</td>
<td>0.015328</td>
<td>5.819517</td>
<td>0.988361</td>
</tr>
<tr>
<td>H</td>
<td>-2.404686</td>
<td>4.439474</td>
<td>0.170737</td>
</tr>
<tr>
<td>H</td>
<td>3.625809</td>
<td>2.276838</td>
<td>-2.044632</td>
</tr>
<tr>
<td>O</td>
<td>2.705258</td>
<td>2.058025</td>
<td>-2.229145</td>
</tr>
<tr>
<td>H</td>
<td>2.175228</td>
<td>2.960702</td>
<td>-2.221144</td>
</tr>
</tbody>
</table>
Table S34: B3LYP 6-311+g* TS2 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.822329</td>
<td>0.817870</td>
<td>-0.215847</td>
</tr>
<tr>
<td>C</td>
<td>-0.783029</td>
<td>1.712201</td>
<td>-0.333769</td>
</tr>
<tr>
<td>C</td>
<td>0.574749</td>
<td>1.248318</td>
<td>-0.330329</td>
</tr>
<tr>
<td>C</td>
<td>0.836812</td>
<td>-0.169439</td>
<td>-0.266118</td>
</tr>
<tr>
<td>C</td>
<td>2.153310</td>
<td>-0.716509</td>
<td>-0.334918</td>
</tr>
<tr>
<td>C</td>
<td>2.370821</td>
<td>-2.063105</td>
<td>-0.259761</td>
</tr>
<tr>
<td>C</td>
<td>1.293149</td>
<td>-2.988307</td>
<td>-0.119109</td>
</tr>
<tr>
<td>C</td>
<td>1.496964</td>
<td>-4.377752</td>
<td>-0.035063</td>
</tr>
<tr>
<td>C</td>
<td>0.419595</td>
<td>-5.246043</td>
<td>0.093737</td>
</tr>
<tr>
<td>C</td>
<td>-0.882805</td>
<td>-4.750347</td>
<td>0.137375</td>
</tr>
<tr>
<td>C</td>
<td>-1.130334</td>
<td>-3.372495</td>
<td>0.053812</td>
</tr>
<tr>
<td>C</td>
<td>-2.457119</td>
<td>-2.833164</td>
<td>0.090930</td>
</tr>
<tr>
<td>C</td>
<td>-2.678751</td>
<td>-1.491013</td>
<td>0.005046</td>
</tr>
<tr>
<td>C</td>
<td>-1.593306</td>
<td>-0.569860</td>
<td>-0.121888</td>
</tr>
<tr>
<td>C</td>
<td>-0.256441</td>
<td>-1.070652</td>
<td>-0.153394</td>
</tr>
<tr>
<td>C</td>
<td>-0.031285</td>
<td>-2.475354</td>
<td>-0.072836</td>
</tr>
<tr>
<td>C</td>
<td>1.623050</td>
<td>2.181741</td>
<td>-0.293655</td>
</tr>
<tr>
<td>C</td>
<td>1.384472</td>
<td>3.701350</td>
<td>-0.344392</td>
</tr>
<tr>
<td>C</td>
<td>0.021336</td>
<td>3.965141</td>
<td>0.341537</td>
</tr>
<tr>
<td>C</td>
<td>-1.059980</td>
<td>3.191957</td>
<td>-0.408154</td>
</tr>
<tr>
<td>O</td>
<td>1.419802</td>
<td>4.153451</td>
<td>-1.650503</td>
</tr>
<tr>
<td>O</td>
<td>-0.354737</td>
<td>5.340055</td>
<td>0.301384</td>
</tr>
<tr>
<td>O</td>
<td>-2.357937</td>
<td>3.471988</td>
<td>0.107308</td>
</tr>
<tr>
<td>H</td>
<td>-2.838133</td>
<td>1.186846</td>
<td>-0.180703</td>
</tr>
<tr>
<td>H</td>
<td>3.001043</td>
<td>-0.061315</td>
<td>-0.470870</td>
</tr>
<tr>
<td>H</td>
<td>3.383265</td>
<td>-2.446999</td>
<td>-0.315418</td>
</tr>
<tr>
<td>H</td>
<td>2.507709</td>
<td>-4.767619</td>
<td>-0.072031</td>
</tr>
<tr>
<td>H</td>
<td>0.591516</td>
<td>-6.313454</td>
<td>0.158859</td>
</tr>
<tr>
<td>H</td>
<td>-1.718626</td>
<td>-5.433503</td>
<td>0.236580</td>
</tr>
<tr>
<td>H</td>
<td>-3.292879</td>
<td>-3.516975</td>
<td>0.187438</td>
</tr>
<tr>
<td>H</td>
<td>-3.689143</td>
<td>-1.100523</td>
<td>0.032094</td>
</tr>
<tr>
<td>H</td>
<td>2.595055</td>
<td>1.849571</td>
<td>0.037045</td>
</tr>
<tr>
<td>H</td>
<td>2.164422</td>
<td>4.172247</td>
<td>0.279865</td>
</tr>
<tr>
<td>H</td>
<td>0.049538</td>
<td>3.627682</td>
<td>1.384100</td>
</tr>
<tr>
<td>H</td>
<td>-1.007865</td>
<td>3.506393</td>
<td>-1.457274</td>
</tr>
<tr>
<td>H</td>
<td>0.046394</td>
<td>5.807835</td>
<td>1.041058</td>
</tr>
<tr>
<td>H</td>
<td>-2.415947</td>
<td>4.432443</td>
<td>0.191328</td>
</tr>
<tr>
<td>H</td>
<td>3.445521</td>
<td>2.148472</td>
<td>-2.287367</td>
</tr>
<tr>
<td>O</td>
<td>2.484024</td>
<td>2.084462</td>
<td>-2.331778</td>
</tr>
<tr>
<td>H</td>
<td>2.077016</td>
<td>3.075317</td>
<td>-2.253843</td>
</tr>
</tbody>
</table>
Table S35: B3LYP 6-311g* **TS2** coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.837842</td>
<td>0.817124</td>
<td>-0.191065</td>
</tr>
<tr>
<td>C</td>
<td>-0.800353</td>
<td>1.712607</td>
<td>-0.335322</td>
</tr>
<tr>
<td>C</td>
<td>0.558462</td>
<td>1.247751</td>
<td>-0.341183</td>
</tr>
<tr>
<td>C</td>
<td>0.818475</td>
<td>-0.169840</td>
<td>-0.297666</td>
</tr>
<tr>
<td>C</td>
<td>2.132251</td>
<td>-0.711563</td>
<td>-0.420491</td>
</tr>
<tr>
<td>C</td>
<td>2.354328</td>
<td>-2.058602</td>
<td>-0.354595</td>
</tr>
<tr>
<td>C</td>
<td>1.283864</td>
<td>-2.984430</td>
<td>-0.170219</td>
</tr>
<tr>
<td>C</td>
<td>1.491259</td>
<td>-4.374017</td>
<td>-0.090783</td>
</tr>
<tr>
<td>C</td>
<td>0.419732</td>
<td>-5.243147</td>
<td>0.074246</td>
</tr>
<tr>
<td>C</td>
<td>-0.881853</td>
<td>-4.750190</td>
<td>0.157774</td>
</tr>
<tr>
<td>C</td>
<td>-1.135039</td>
<td>-3.372932</td>
<td>0.079070</td>
</tr>
<tr>
<td>C</td>
<td>-2.460586</td>
<td>-2.834517</td>
<td>0.153789</td>
</tr>
<tr>
<td>C</td>
<td>-2.687076</td>
<td>-1.492602</td>
<td>0.069501</td>
</tr>
<tr>
<td>C</td>
<td>-1.608074</td>
<td>-0.569228</td>
<td>-0.090848</td>
</tr>
<tr>
<td>C</td>
<td>-0.271214</td>
<td>-1.070580</td>
<td>-0.156243</td>
</tr>
<tr>
<td>C</td>
<td>-0.040986</td>
<td>-2.474085</td>
<td>-0.082493</td>
</tr>
<tr>
<td>C</td>
<td>1.600320</td>
<td>2.183097</td>
<td>-0.228786</td>
</tr>
<tr>
<td>C</td>
<td>1.357425</td>
<td>3.683664</td>
<td>-0.364122</td>
</tr>
<tr>
<td>C</td>
<td>-0.000763</td>
<td>3.973360</td>
<td>0.328624</td>
</tr>
<tr>
<td>C</td>
<td>-1.075810</td>
<td>3.186673</td>
<td>-0.420538</td>
</tr>
<tr>
<td>O</td>
<td>1.333425</td>
<td>4.016433</td>
<td>-1.698717</td>
</tr>
<tr>
<td>O</td>
<td>-0.373512</td>
<td>5.345228</td>
<td>0.237335</td>
</tr>
<tr>
<td>O</td>
<td>-2.375830</td>
<td>3.483264</td>
<td>0.070704</td>
</tr>
<tr>
<td>H</td>
<td>-2.852437</td>
<td>1.191070</td>
<td>-0.137273</td>
</tr>
<tr>
<td>H</td>
<td>2.961466</td>
<td>-0.045726</td>
<td>-0.614647</td>
</tr>
<tr>
<td>H</td>
<td>3.364344</td>
<td>-2.443194</td>
<td>-0.454368</td>
</tr>
<tr>
<td>H</td>
<td>2.501755</td>
<td>-4.763094</td>
<td>-0.160448</td>
</tr>
<tr>
<td>H</td>
<td>0.595654</td>
<td>-6.312399</td>
<td>0.136013</td>
</tr>
<tr>
<td>H</td>
<td>-1.713607</td>
<td>-5.435465</td>
<td>0.284610</td>
</tr>
<tr>
<td>H</td>
<td>-3.292867</td>
<td>-3.520141</td>
<td>0.276435</td>
</tr>
<tr>
<td>H</td>
<td>-3.698261</td>
<td>-1.103596</td>
<td>0.122849</td>
</tr>
<tr>
<td>H</td>
<td>2.550217</td>
<td>1.845946</td>
<td>0.161633</td>
</tr>
<tr>
<td>H</td>
<td>2.142950</td>
<td>4.220758</td>
<td>0.203422</td>
</tr>
<tr>
<td>H</td>
<td>0.016316</td>
<td>3.659057</td>
<td>1.380140</td>
</tr>
<tr>
<td>H</td>
<td>-0.984190</td>
<td>3.493832</td>
<td>-1.471834</td>
</tr>
<tr>
<td>H</td>
<td>-0.013275</td>
<td>5.818844</td>
<td>0.994729</td>
</tr>
<tr>
<td>H</td>
<td>-2.402718</td>
<td>4.446602</td>
<td>0.151447</td>
</tr>
<tr>
<td>H</td>
<td>3.656166</td>
<td>2.296420</td>
<td>-2.007190</td>
</tr>
<tr>
<td>O</td>
<td>2.743003</td>
<td>2.060340</td>
<td>-2.214652</td>
</tr>
<tr>
<td>H</td>
<td>2.193862</td>
<td>2.957026</td>
<td>-2.208359</td>
</tr>
</tbody>
</table>
Table S36: B3LYP 6-311+g* TS2 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.823875</td>
<td>0.818238</td>
<td>-0.215115</td>
</tr>
<tr>
<td>C</td>
<td>-0.784598</td>
<td>1.712684</td>
<td>-0.335847</td>
</tr>
<tr>
<td>C</td>
<td>0.574657</td>
<td>1.249014</td>
<td>-0.332237</td>
</tr>
<tr>
<td>C</td>
<td>0.836013</td>
<td>-0.170344</td>
<td>-0.270228</td>
</tr>
<tr>
<td>C</td>
<td>2.151293</td>
<td>-0.716992</td>
<td>-0.343637</td>
</tr>
<tr>
<td>C</td>
<td>2.369435</td>
<td>-2.064986</td>
<td>-0.268331</td>
</tr>
<tr>
<td>C</td>
<td>1.292507</td>
<td>-2.989226</td>
<td>-0.123059</td>
</tr>
<tr>
<td>C</td>
<td>1.496153</td>
<td>-4.379467</td>
<td>-0.037931</td>
</tr>
<tr>
<td>C</td>
<td>0.418763</td>
<td>-5.247644</td>
<td>0.095355</td>
</tr>
<tr>
<td>C</td>
<td>-0.883831</td>
<td>-4.751688</td>
<td>0.142278</td>
</tr>
<tr>
<td>C</td>
<td>-1.131894</td>
<td>-3.373188</td>
<td>0.057685</td>
</tr>
<tr>
<td>C</td>
<td>-2.457873</td>
<td>-2.834118</td>
<td>0.097897</td>
</tr>
<tr>
<td>C</td>
<td>-2.679788</td>
<td>-1.490585</td>
<td>0.010933</td>
</tr>
<tr>
<td>C</td>
<td>-1.595331</td>
<td>-0.570213</td>
<td>-0.119689</td>
</tr>
<tr>
<td>C</td>
<td>-0.257759</td>
<td>1.071467</td>
<td>-0.154119</td>
</tr>
<tr>
<td>C</td>
<td>-0.032553</td>
<td>-2.475775</td>
<td>-0.073223</td>
</tr>
<tr>
<td>C</td>
<td>1.621385</td>
<td>2.181671</td>
<td>-0.285981</td>
</tr>
<tr>
<td>C</td>
<td>1.383480</td>
<td>3.698041</td>
<td>-0.339949</td>
</tr>
<tr>
<td>C</td>
<td>0.018766</td>
<td>3.964675</td>
<td>0.343296</td>
</tr>
<tr>
<td>C</td>
<td>-1.060031</td>
<td>3.193127</td>
<td>-0.411597</td>
</tr>
<tr>
<td>O</td>
<td>1.416327</td>
<td>4.142997</td>
<td>-1.650541</td>
</tr>
<tr>
<td>O</td>
<td>-0.355765</td>
<td>5.340699</td>
<td>0.299850</td>
</tr>
<tr>
<td>O</td>
<td>-2.361517</td>
<td>3.475416</td>
<td>0.094383</td>
</tr>
<tr>
<td>H</td>
<td>-2.840610</td>
<td>1.188227</td>
<td>-0.178745</td>
</tr>
<tr>
<td>H</td>
<td>2.998865</td>
<td>-0.060497</td>
<td>-0.484236</td>
</tr>
<tr>
<td>H</td>
<td>3.382703</td>
<td>-2.449391</td>
<td>-0.327639</td>
</tr>
<tr>
<td>H</td>
<td>2.507821</td>
<td>-4.769840</td>
<td>-0.077645</td>
</tr>
<tr>
<td>H</td>
<td>0.590945</td>
<td>-6.316094</td>
<td>0.161419</td>
</tr>
<tr>
<td>H</td>
<td>-1.720369</td>
<td>-5.435260</td>
<td>0.244984</td>
</tr>
<tr>
<td>H</td>
<td>-3.294425</td>
<td>-3.518326</td>
<td>0.197562</td>
</tr>
<tr>
<td>H</td>
<td>-3.691293</td>
<td>-1.099906</td>
<td>0.040164</td>
</tr>
<tr>
<td>H</td>
<td>2.594903</td>
<td>1.847157</td>
<td>0.042379</td>
</tr>
<tr>
<td>H</td>
<td>2.162875</td>
<td>4.176070</td>
<td>0.281539</td>
</tr>
<tr>
<td>H</td>
<td>0.043722</td>
<td>3.627408</td>
<td>1.387095</td>
</tr>
<tr>
<td>H</td>
<td>-0.998061</td>
<td>3.506118</td>
<td>-1.461807</td>
</tr>
<tr>
<td>H</td>
<td>0.024962</td>
<td>5.803759</td>
<td>1.055212</td>
</tr>
<tr>
<td>H</td>
<td>-2.413044</td>
<td>4.437971</td>
<td>0.180978</td>
</tr>
<tr>
<td>H</td>
<td>3.471055</td>
<td>2.166263</td>
<td>-2.283415</td>
</tr>
<tr>
<td>O</td>
<td>2.509512</td>
<td>2.089082</td>
<td>-2.340368</td>
</tr>
<tr>
<td>H</td>
<td>2.085455</td>
<td>3.079101</td>
<td>-2.247194</td>
</tr>
</tbody>
</table>
Table S37: BPW91 6-311g* **TS3** coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.457528</td>
<td>4.173041</td>
<td>1.334696</td>
</tr>
<tr>
<td>C</td>
<td>0.025677</td>
<td>2.755641</td>
<td>1.576078</td>
</tr>
<tr>
<td>C</td>
<td>0.552723</td>
<td>1.739238</td>
<td>0.688729</td>
</tr>
<tr>
<td>C</td>
<td>1.688434</td>
<td>2.012423</td>
<td>-0.065183</td>
</tr>
<tr>
<td>C</td>
<td>2.343792</td>
<td>3.352229</td>
<td>-0.120336</td>
</tr>
<tr>
<td>C</td>
<td>1.969656</td>
<td>4.276250</td>
<td>1.037827</td>
</tr>
<tr>
<td>C</td>
<td>-0.029809</td>
<td>0.403428</td>
<td>0.711427</td>
</tr>
<tr>
<td>C</td>
<td>-0.972324</td>
<td>0.089204</td>
<td>1.737973</td>
</tr>
<tr>
<td>C</td>
<td>-1.379113</td>
<td>1.095377</td>
<td>2.680766</td>
</tr>
<tr>
<td>C</td>
<td>-0.884665</td>
<td>2.423718</td>
<td>2.554408</td>
</tr>
<tr>
<td>C</td>
<td>-1.523011</td>
<td>-1.223552</td>
<td>1.828390</td>
</tr>
<tr>
<td>C</td>
<td>-1.148999</td>
<td>-2.222757</td>
<td>0.877971</td>
</tr>
<tr>
<td>C</td>
<td>-0.229604</td>
<td>-1.867161</td>
<td>-0.155009</td>
</tr>
<tr>
<td>C</td>
<td>0.315796</td>
<td>-0.603155</td>
<td>-0.237077</td>
</tr>
<tr>
<td>C</td>
<td>-2.452466</td>
<td>-1.546112</td>
<td>2.868167</td>
</tr>
<tr>
<td>C</td>
<td>-2.978597</td>
<td>-2.853958</td>
<td>2.939874</td>
</tr>
<tr>
<td>C</td>
<td>-2.606756</td>
<td>-3.828319</td>
<td>2.006628</td>
</tr>
<tr>
<td>C</td>
<td>-1.706164</td>
<td>-3.519409</td>
<td>0.985586</td>
</tr>
<tr>
<td>C</td>
<td>-2.308233</td>
<td>0.748955</td>
<td>3.705929</td>
</tr>
<tr>
<td>C</td>
<td>-2.821701</td>
<td>-0.524959</td>
<td>3.800495</td>
</tr>
<tr>
<td>O</td>
<td>1.754082</td>
<td>3.851567</td>
<td>-1.320115</td>
</tr>
<tr>
<td>O</td>
<td>2.298073</td>
<td>5.628384</td>
<td>0.713218</td>
</tr>
<tr>
<td>O</td>
<td>0.091896</td>
<td>5.018005</td>
<td>2.419717</td>
</tr>
<tr>
<td>O</td>
<td>3.120419</td>
<td>3.061718</td>
<td>-3.187644</td>
</tr>
<tr>
<td>As</td>
<td>2.800552</td>
<td>1.446610</td>
<td>-3.736379</td>
</tr>
<tr>
<td>O</td>
<td>2.611610</td>
<td>0.302736</td>
<td>-2.509378</td>
</tr>
<tr>
<td>C</td>
<td>1.210210</td>
<td>1.516608</td>
<td>-4.879529</td>
</tr>
<tr>
<td>C</td>
<td>4.312295</td>
<td>1.014308</td>
<td>-4.897423</td>
</tr>
<tr>
<td>H</td>
<td>-1.249034</td>
<td>3.195742</td>
<td>3.235797</td>
</tr>
<tr>
<td>H</td>
<td>1.002744</td>
<td>-0.370270</td>
<td>-1.055841</td>
</tr>
<tr>
<td>H</td>
<td>0.039384</td>
<td>-2.619644</td>
<td>-0.899688</td>
</tr>
<tr>
<td>H</td>
<td>-1.422511</td>
<td>-4.281787</td>
<td>0.256926</td>
</tr>
<tr>
<td>H</td>
<td>-3.025254</td>
<td>-4.833436</td>
<td>2.076543</td>
</tr>
<tr>
<td>H</td>
<td>-3.685980</td>
<td>-3.099988</td>
<td>3.734524</td>
</tr>
<tr>
<td>H</td>
<td>-3.530064</td>
<td>-0.770089</td>
<td>4.594824</td>
</tr>
<tr>
<td>H</td>
<td>-2.611456</td>
<td>1.516621</td>
<td>4.420105</td>
</tr>
<tr>
<td>H</td>
<td>2.120035</td>
<td>1.257331</td>
<td>-0.736451</td>
</tr>
<tr>
<td>H</td>
<td>3.441411</td>
<td>3.275132</td>
<td>-0.211924</td>
</tr>
<tr>
<td>H</td>
<td>2.530955</td>
<td>4.018914</td>
<td>1.948858</td>
</tr>
<tr>
<td>H</td>
<td>-0.056939</td>
<td>4.500792</td>
<td>0.407007</td>
</tr>
<tr>
<td>H</td>
<td>2.054167</td>
<td>5.714348</td>
<td>-0.233176</td>
</tr>
<tr>
<td>H</td>
<td>0.492823</td>
<td>5.882681</td>
<td>2.211635</td>
</tr>
<tr>
<td>H</td>
<td>1.362114</td>
<td>2.250891</td>
<td>-5.680087</td>
</tr>
<tr>
<td>H</td>
<td>0.354398</td>
<td>1.815902</td>
<td>-4.262319</td>
</tr>
<tr>
<td>H</td>
<td>1.023483</td>
<td>0.525615</td>
<td>-5.311381</td>
</tr>
<tr>
<td>H</td>
<td>4.404021</td>
<td>1.777025</td>
<td>-5.680073</td>
</tr>
<tr>
<td>H</td>
<td>2.387514</td>
<td>3.451810</td>
<td>-2.231052</td>
</tr>
<tr>
<td>H</td>
<td>4.149009</td>
<td>0.029410</td>
<td>-5.352010</td>
</tr>
<tr>
<td>H</td>
<td>5.223859</td>
<td>0.995175</td>
<td>-4.288483</td>
</tr>
</tbody>
</table>
Table S38: BPW91 6-311+g* TS3 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.530483</td>
<td>4.181033</td>
<td>1.436597</td>
</tr>
<tr>
<td>C</td>
<td>0.062397</td>
<td>2.758405</td>
<td>1.616256</td>
</tr>
<tr>
<td>C</td>
<td>0.552736</td>
<td>1.753280</td>
<td>0.701981</td>
</tr>
<tr>
<td>C</td>
<td>1.656153</td>
<td>2.037097</td>
<td>-0.107213</td>
</tr>
<tr>
<td>C</td>
<td>2.280871</td>
<td>3.386161</td>
<td>-0.190657</td>
</tr>
<tr>
<td>C</td>
<td>2.011789</td>
<td>4.249012</td>
<td>1.042823</td>
</tr>
<tr>
<td>C</td>
<td>-0.038666</td>
<td>0.425258</td>
<td>0.716246</td>
</tr>
<tr>
<td>C</td>
<td>-0.986120</td>
<td>0.108467</td>
<td>1.739173</td>
</tr>
<tr>
<td>C</td>
<td>-1.380315</td>
<td>1.107866</td>
<td>2.691675</td>
</tr>
<tr>
<td>C</td>
<td>-0.857417</td>
<td>2.426125</td>
<td>2.588324</td>
</tr>
<tr>
<td>C</td>
<td>-1.553701</td>
<td>-1.198760</td>
<td>1.814932</td>
</tr>
<tr>
<td>C</td>
<td>-1.187632</td>
<td>-2.194415</td>
<td>0.857406</td>
</tr>
<tr>
<td>C</td>
<td>-0.258876</td>
<td>-1.839566</td>
<td>-0.169014</td>
</tr>
<tr>
<td>C</td>
<td>0.298951</td>
<td>-0.581629</td>
<td>-0.238153</td>
</tr>
<tr>
<td>C</td>
<td>-2.491362</td>
<td>-1.519678</td>
<td>2.848478</td>
</tr>
<tr>
<td>C</td>
<td>-3.033985</td>
<td>-2.821909</td>
<td>2.905681</td>
</tr>
<tr>
<td>C</td>
<td>-2.669034</td>
<td>-3.792173</td>
<td>1.965556</td>
</tr>
<tr>
<td>C</td>
<td>-1.759063</td>
<td>-3.484973</td>
<td>0.951067</td>
</tr>
<tr>
<td>C</td>
<td>-2.318241</td>
<td>0.763966</td>
<td>3.711450</td>
</tr>
<tr>
<td>C</td>
<td>-2.850649</td>
<td>-0.502801</td>
<td>3.790314</td>
</tr>
<tr>
<td>O</td>
<td>1.526856</td>
<td>3.769074</td>
<td>-1.338799</td>
</tr>
<tr>
<td>O</td>
<td>2.303527</td>
<td>5.639530</td>
<td>0.832633</td>
</tr>
<tr>
<td>O</td>
<td>0.272357</td>
<td>4.946651</td>
<td>2.614284</td>
</tr>
<tr>
<td>O</td>
<td>2.720617</td>
<td>3.101991</td>
<td>-3.371503</td>
</tr>
<tr>
<td>As</td>
<td>2.693364</td>
<td>1.435124</td>
<td>-3.874518</td>
</tr>
<tr>
<td>O</td>
<td>2.601495</td>
<td>0.320976</td>
<td>-2.602121</td>
</tr>
<tr>
<td>C</td>
<td>1.182137</td>
<td>1.219491</td>
<td>-5.099809</td>
</tr>
<tr>
<td>C</td>
<td>4.322605</td>
<td>1.199900</td>
<td>-4.925771</td>
</tr>
<tr>
<td>H</td>
<td>-1.201560</td>
<td>3.189425</td>
<td>3.286666</td>
</tr>
<tr>
<td>H</td>
<td>0.993119</td>
<td>-0.355141</td>
<td>-1.051351</td>
</tr>
<tr>
<td>H</td>
<td>0.007115</td>
<td>-2.589289</td>
<td>-0.917976</td>
</tr>
<tr>
<td>H</td>
<td>-1.480116</td>
<td>-4.244674</td>
<td>0.217446</td>
</tr>
<tr>
<td>H</td>
<td>-3.099476</td>
<td>-4.793285</td>
<td>2.024503</td>
</tr>
<tr>
<td>H</td>
<td>-3.747925</td>
<td>-3.066952</td>
<td>3.695177</td>
</tr>
<tr>
<td>H</td>
<td>-3.565415</td>
<td>-0.746376</td>
<td>4.579723</td>
</tr>
<tr>
<td>H</td>
<td>-2.611625</td>
<td>1.528003</td>
<td>4.434115</td>
</tr>
<tr>
<td>H</td>
<td>2.058031</td>
<td>1.295505</td>
<td>-0.808690</td>
</tr>
<tr>
<td>H</td>
<td>3.362188</td>
<td>3.346829</td>
<td>-0.405858</td>
</tr>
<tr>
<td>H</td>
<td>2.617670</td>
<td>3.856077</td>
<td>1.878639</td>
</tr>
<tr>
<td>H</td>
<td>-0.042370</td>
<td>4.606802</td>
<td>0.588145</td>
</tr>
<tr>
<td>H</td>
<td>3.243613</td>
<td>5.797894</td>
<td>1.024549</td>
</tr>
<tr>
<td>H</td>
<td>0.689861</td>
<td>5.815512</td>
<td>2.458630</td>
</tr>
<tr>
<td>H</td>
<td>1.260848</td>
<td>1.952807</td>
<td>-5.911848</td>
</tr>
<tr>
<td>H</td>
<td>0.254225</td>
<td>1.383208</td>
<td>-4.538756</td>
</tr>
<tr>
<td>H</td>
<td>1.192484</td>
<td>0.202332</td>
<td>-5.510774</td>
</tr>
<tr>
<td>H</td>
<td>4.339253</td>
<td>1.931866</td>
<td>-5.742533</td>
</tr>
<tr>
<td>H</td>
<td>2.084957</td>
<td>3.410175</td>
<td>-2.304657</td>
</tr>
<tr>
<td>H</td>
<td>4.344936</td>
<td>0.182295</td>
<td>-5.334499</td>
</tr>
<tr>
<td>H</td>
<td>5.185694</td>
<td>1.355629</td>
<td>-4.267650</td>
</tr>
<tr>
<td>Atom</td>
<td>x</td>
<td>y</td>
<td>z</td>
</tr>
<tr>
<td>------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>C</td>
<td>0.508636</td>
<td>4.193509</td>
<td>1.405595</td>
</tr>
<tr>
<td>C</td>
<td>0.047507</td>
<td>2.762264</td>
<td>1.593409</td>
</tr>
<tr>
<td>C</td>
<td>0.560057</td>
<td>1.749415</td>
<td>0.691495</td>
</tr>
<tr>
<td>C</td>
<td>1.683486</td>
<td>2.032247</td>
<td>-0.098259</td>
</tr>
<tr>
<td>C</td>
<td>2.302145</td>
<td>3.391376</td>
<td>-0.185734</td>
</tr>
<tr>
<td>C</td>
<td>2.001583</td>
<td>4.271859</td>
<td>1.035519</td>
</tr>
<tr>
<td>C</td>
<td>-0.029087</td>
<td>0.414978</td>
<td>0.707983</td>
</tr>
<tr>
<td>C</td>
<td>-0.985514</td>
<td>0.099523</td>
<td>1.730207</td>
</tr>
<tr>
<td>C</td>
<td>-1.394452</td>
<td>1.106922</td>
<td>2.675681</td>
</tr>
<tr>
<td>C</td>
<td>-0.880321</td>
<td>2.431368</td>
<td>2.561665</td>
</tr>
<tr>
<td>C</td>
<td>-1.546764</td>
<td>-1.215164</td>
<td>1.813158</td>
</tr>
<tr>
<td>C</td>
<td>-1.169811</td>
<td>-2.218226</td>
<td>0.860179</td>
</tr>
<tr>
<td>C</td>
<td>-0.238360</td>
<td>-1.860977</td>
<td>-0.169208</td>
</tr>
<tr>
<td>C</td>
<td>0.314048</td>
<td>-0.598600</td>
<td>-0.245672</td>
</tr>
<tr>
<td>C</td>
<td>-2.490720</td>
<td>-1.535937</td>
<td>2.848060</td>
</tr>
<tr>
<td>C</td>
<td>-3.025075</td>
<td>-2.844938</td>
<td>2.911686</td>
</tr>
<tr>
<td>C</td>
<td>-2.648887</td>
<td>-3.820916</td>
<td>1.977525</td>
</tr>
<tr>
<td>C</td>
<td>-1.735506</td>
<td>-3.514402</td>
<td>0.961732</td>
</tr>
<tr>
<td>C</td>
<td>-2.338656</td>
<td>0.761690</td>
<td>3.695361</td>
</tr>
<tr>
<td>C</td>
<td>-2.862542</td>
<td>-0.510231</td>
<td>3.782272</td>
</tr>
<tr>
<td>O</td>
<td>1.555183</td>
<td>3.760856</td>
<td>-1.954144</td>
</tr>
<tr>
<td>O</td>
<td>2.274996</td>
<td>5.672546</td>
<td>0.804054</td>
</tr>
<tr>
<td>O</td>
<td>0.231500</td>
<td>4.973358</td>
<td>2.579249</td>
</tr>
<tr>
<td>As</td>
<td>2.718351</td>
<td>1.432896</td>
<td>-3.829207</td>
</tr>
<tr>
<td>O</td>
<td>2.588192</td>
<td>0.297240</td>
<td>-2.575205</td>
</tr>
<tr>
<td>C</td>
<td>1.146496</td>
<td>1.351340</td>
<td>-5.029207</td>
</tr>
<tr>
<td>C</td>
<td>4.302987</td>
<td>1.098622</td>
<td>-4.958593</td>
</tr>
<tr>
<td>H</td>
<td>-1.234175</td>
<td>3.199663</td>
<td>3.248579</td>
</tr>
<tr>
<td>H</td>
<td>1.002323</td>
<td>-0.370702</td>
<td>-1.062481</td>
</tr>
<tr>
<td>H</td>
<td>0.031152</td>
<td>-2.612600</td>
<td>-0.914465</td>
</tr>
<tr>
<td>H</td>
<td>-1.450157</td>
<td>-4.277408</td>
<td>0.234680</td>
</tr>
<tr>
<td>H</td>
<td>-3.072730</td>
<td>-4.824138</td>
<td>2.041824</td>
</tr>
<tr>
<td>H</td>
<td>-3.740209</td>
<td>-3.089913</td>
<td>3.699483</td>
</tr>
<tr>
<td>H</td>
<td>-3.579522</td>
<td>-0.752588</td>
<td>4.569477</td>
</tr>
<tr>
<td>H</td>
<td>-2.641765</td>
<td>1.529563</td>
<td>4.409305</td>
</tr>
<tr>
<td>H</td>
<td>2.106554</td>
<td>1.283002</td>
<td>-0.775740</td>
</tr>
<tr>
<td>H</td>
<td>3.385320</td>
<td>3.361793</td>
<td>-0.389410</td>
</tr>
<tr>
<td>H</td>
<td>2.593525</td>
<td>3.903021</td>
<td>1.891296</td>
</tr>
<tr>
<td>H</td>
<td>-0.049201</td>
<td>4.608058</td>
<td>0.542706</td>
</tr>
<tr>
<td>H</td>
<td>3.210732</td>
<td>5.841776</td>
<td>1.013479</td>
</tr>
<tr>
<td>H</td>
<td>0.662249</td>
<td>5.835563</td>
<td>2.412257</td>
</tr>
<tr>
<td>H</td>
<td>1.261768</td>
<td>2.085817</td>
<td>-5.835724</td>
</tr>
<tr>
<td>H</td>
<td>0.251369</td>
<td>1.586035</td>
<td>-4.440547</td>
</tr>
<tr>
<td>H</td>
<td>1.057087</td>
<td>0.342398</td>
<td>-5.450575</td>
</tr>
<tr>
<td>H</td>
<td>4.353232</td>
<td>1.855833</td>
<td>-5.750263</td>
</tr>
<tr>
<td>H</td>
<td>2.167693</td>
<td>3.419340</td>
<td>-2.297954</td>
</tr>
<tr>
<td>H</td>
<td>4.226493</td>
<td>0.097839</td>
<td>-5.400802</td>
</tr>
<tr>
<td>H</td>
<td>5.197779</td>
<td>1.158449</td>
<td>-4.327965</td>
</tr>
</tbody>
</table>
Table S40: BLYP 6-311+g* TS3 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.526337</td>
<td>4.184340</td>
<td>1.444813</td>
</tr>
<tr>
<td>C</td>
<td>0.050763</td>
<td>2.754535</td>
<td>1.625800</td>
</tr>
<tr>
<td>C</td>
<td>0.551268</td>
<td>1.739202</td>
<td>0.716574</td>
</tr>
<tr>
<td>C</td>
<td>1.657976</td>
<td>2.019726</td>
<td>-0.090611</td>
</tr>
<tr>
<td>C</td>
<td>2.283584</td>
<td>3.376576</td>
<td>-0.193195</td>
</tr>
<tr>
<td>C</td>
<td>2.012574</td>
<td>4.248954</td>
<td>1.045130</td>
</tr>
<tr>
<td>C</td>
<td>-0.044425</td>
<td>0.404766</td>
<td>0.738089</td>
</tr>
<tr>
<td>C</td>
<td>-1.000360</td>
<td>0.094513</td>
<td>1.761482</td>
</tr>
<tr>
<td>C</td>
<td>-1.402131</td>
<td>1.104659</td>
<td>2.706417</td>
</tr>
<tr>
<td>C</td>
<td>-0.877563</td>
<td>2.426950</td>
<td>2.593956</td>
</tr>
<tr>
<td>C</td>
<td>-1.569450</td>
<td>-1.216865</td>
<td>1.845899</td>
</tr>
<tr>
<td>C</td>
<td>-1.198501</td>
<td>-2.223237</td>
<td>0.894555</td>
</tr>
<tr>
<td>C</td>
<td>-0.263979</td>
<td>-1.873739</td>
<td>-0.134005</td>
</tr>
<tr>
<td>C</td>
<td>0.294759</td>
<td>-0.612973</td>
<td>-0.210621</td>
</tr>
<tr>
<td>C</td>
<td>-2.514833</td>
<td>-1.530951</td>
<td>2.881356</td>
</tr>
<tr>
<td>C</td>
<td>-3.057583</td>
<td>-2.837110</td>
<td>2.940762</td>
</tr>
<tr>
<td>C</td>
<td>-2.687197</td>
<td>-3.817146</td>
<td>2.013561</td>
</tr>
<tr>
<td>C</td>
<td>-1.771587</td>
<td>-3.516954</td>
<td>0.997340</td>
</tr>
<tr>
<td>C</td>
<td>-2.347502</td>
<td>0.767075</td>
<td>3.726682</td>
</tr>
<tr>
<td>C</td>
<td>-2.880044</td>
<td>-5.026255</td>
<td>3.814782</td>
</tr>
<tr>
<td>O</td>
<td>1.558371</td>
<td>3.779731</td>
<td>-1.359548</td>
</tr>
<tr>
<td>O</td>
<td>2.310257</td>
<td>5.649970</td>
<td>0.826347</td>
</tr>
<tr>
<td>O</td>
<td>0.273578</td>
<td>4.948612</td>
<td>2.641389</td>
</tr>
<tr>
<td>O</td>
<td>2.753449</td>
<td>3.122777</td>
<td>-3.403097</td>
</tr>
<tr>
<td>As</td>
<td>2.712529</td>
<td>1.445312</td>
<td>-3.933752</td>
</tr>
<tr>
<td>O</td>
<td>2.592966</td>
<td>0.312534</td>
<td>-2.669207</td>
</tr>
<tr>
<td>C</td>
<td>1.196617</td>
<td>1.274002</td>
<td>-5.182055</td>
</tr>
<tr>
<td>C</td>
<td>4.369206</td>
<td>1.224724</td>
<td>-4.978111</td>
</tr>
<tr>
<td>H</td>
<td>-1.227608</td>
<td>3.193223</td>
<td>3.284875</td>
</tr>
<tr>
<td>H</td>
<td>0.988784</td>
<td>-0.393753</td>
<td>-1.023479</td>
</tr>
<tr>
<td>H</td>
<td>0.004839</td>
<td>-2.627659</td>
<td>-0.876798</td>
</tr>
<tr>
<td>H</td>
<td>-1.490160</td>
<td>-4.282459</td>
<td>0.271389</td>
</tr>
<tr>
<td>H</td>
<td>-3.116920</td>
<td>-8.177544</td>
<td>2.079114</td>
</tr>
<tr>
<td>H</td>
<td>-3.774082</td>
<td>-3.076984</td>
<td>3.734877</td>
</tr>
<tr>
<td>H</td>
<td>-3.598040</td>
<td>-0.793071</td>
<td>4.602759</td>
</tr>
<tr>
<td>H</td>
<td>-2.645695</td>
<td>1.536663</td>
<td>4.440826</td>
</tr>
<tr>
<td>H</td>
<td>2.062249</td>
<td>1.272246</td>
<td>-0.778203</td>
</tr>
<tr>
<td>H</td>
<td>3.369110</td>
<td>3.325891</td>
<td>-0.387228</td>
</tr>
<tr>
<td>H</td>
<td>2.621757</td>
<td>3.895832</td>
<td>1.881725</td>
</tr>
<tr>
<td>H</td>
<td>-0.051635</td>
<td>4.623180</td>
<td>0.609170</td>
</tr>
<tr>
<td>H</td>
<td>3.255987</td>
<td>5.806352</td>
<td>1.006345</td>
</tr>
<tr>
<td>H</td>
<td>0.674601</td>
<td>5.827873</td>
<td>2.487140</td>
</tr>
<tr>
<td>H</td>
<td>1.294589</td>
<td>2.026305</td>
<td>-5.981248</td>
</tr>
<tr>
<td>H</td>
<td>0.266678</td>
<td>1.435388</td>
<td>-4.631284</td>
</tr>
<tr>
<td>H</td>
<td>1.202278</td>
<td>0.266371</td>
<td>-5.622611</td>
</tr>
<tr>
<td>H</td>
<td>4.398521</td>
<td>1.978630</td>
<td>-5.773944</td>
</tr>
<tr>
<td>H</td>
<td>2.142244</td>
<td>3.410112</td>
<td>-2.367324</td>
</tr>
<tr>
<td>H</td>
<td>4.387520</td>
<td>0.217733</td>
<td>-5.412196</td>
</tr>
<tr>
<td>H</td>
<td>5.222731</td>
<td>1.357354</td>
<td>-4.303167</td>
</tr>
</tbody>
</table>
Table S41: B3LYP 6-311g* TS3 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.533080</td>
<td>4.166009</td>
<td>1.416147</td>
</tr>
<tr>
<td>C</td>
<td>0.066580</td>
<td>2.743883</td>
<td>1.596641</td>
</tr>
<tr>
<td>C</td>
<td>0.555884</td>
<td>1.740226</td>
<td>0.692504</td>
</tr>
<tr>
<td>C</td>
<td>1.659218</td>
<td>2.024098</td>
<td>-0.112580</td>
</tr>
<tr>
<td>C</td>
<td>2.276598</td>
<td>3.369100</td>
<td>-0.200948</td>
</tr>
<tr>
<td>C</td>
<td>2.005306</td>
<td>4.238497</td>
<td>1.019802</td>
</tr>
<tr>
<td>C</td>
<td>-0.027557</td>
<td>0.419942</td>
<td>0.707198</td>
</tr>
<tr>
<td>C</td>
<td>-0.975646</td>
<td>0.108494</td>
<td>1.721246</td>
</tr>
<tr>
<td>C</td>
<td>-1.374186</td>
<td>1.106969</td>
<td>2.661215</td>
</tr>
<tr>
<td>C</td>
<td>-0.855863</td>
<td>2.419197</td>
<td>2.557483</td>
</tr>
<tr>
<td>C</td>
<td>-1.538646</td>
<td>-1.197038</td>
<td>1.802214</td>
</tr>
<tr>
<td>C</td>
<td>-1.167963</td>
<td>-2.191109</td>
<td>0.856888</td>
</tr>
<tr>
<td>C</td>
<td>-0.237504</td>
<td>-1.837708</td>
<td>-0.167290</td>
</tr>
<tr>
<td>C</td>
<td>0.313531</td>
<td>-0.590309</td>
<td>-0.243521</td>
</tr>
<tr>
<td>C</td>
<td>-2.475180</td>
<td>-1.512320</td>
<td>2.827462</td>
</tr>
<tr>
<td>C</td>
<td>-3.011204</td>
<td>-2.807621</td>
<td>2.890132</td>
</tr>
<tr>
<td>C</td>
<td>-2.641297</td>
<td>-3.777375</td>
<td>1.961791</td>
</tr>
<tr>
<td>C</td>
<td>-1.732379</td>
<td>-3.474693</td>
<td>0.954165</td>
</tr>
<tr>
<td>C</td>
<td>-2.316206</td>
<td>0.766160</td>
<td>3.677142</td>
</tr>
<tr>
<td>C</td>
<td>-2.840838</td>
<td>-0.490373</td>
<td>3.759686</td>
</tr>
<tr>
<td>O</td>
<td>1.507499</td>
<td>3.708563</td>
<td>-1.335167</td>
</tr>
<tr>
<td>O</td>
<td>2.279218</td>
<td>5.618208</td>
<td>0.793148</td>
</tr>
<tr>
<td>O</td>
<td>0.289020</td>
<td>4.917826</td>
<td>2.593069</td>
</tr>
<tr>
<td>O</td>
<td>2.755584</td>
<td>3.084546</td>
<td>-3.309208</td>
</tr>
<tr>
<td>As</td>
<td>2.672986</td>
<td>1.443643</td>
<td>-3.817200</td>
</tr>
<tr>
<td>O</td>
<td>2.546412</td>
<td>0.346366</td>
<td>-2.561900</td>
</tr>
<tr>
<td>C</td>
<td>1.163198</td>
<td>1.295295</td>
<td>-5.035835</td>
</tr>
<tr>
<td>C</td>
<td>5.281419</td>
<td>1.164571</td>
<td>-4.865600</td>
</tr>
<tr>
<td>H</td>
<td>-1.200171</td>
<td>3.179995</td>
<td>3.244778</td>
</tr>
<tr>
<td>H</td>
<td>0.998928</td>
<td>-0.366031</td>
<td>-1.052596</td>
</tr>
<tr>
<td>H</td>
<td>0.028335</td>
<td>-2.585788</td>
<td>-0.905799</td>
</tr>
<tr>
<td>H</td>
<td>-1.451124</td>
<td>-4.232276</td>
<td>0.231742</td>
</tr>
<tr>
<td>H</td>
<td>-3.065763</td>
<td>-4.771785</td>
<td>2.024126</td>
</tr>
<tr>
<td>H</td>
<td>-3.722168</td>
<td>-3.048897</td>
<td>3.671873</td>
</tr>
<tr>
<td>H</td>
<td>-3.553805</td>
<td>-0.730301</td>
<td>4.540257</td>
</tr>
<tr>
<td>H</td>
<td>-2.611164</td>
<td>1.529060</td>
<td>4.387513</td>
</tr>
<tr>
<td>H</td>
<td>2.064180</td>
<td>1.285585</td>
<td>-0.799810</td>
</tr>
<tr>
<td>H</td>
<td>3.348092</td>
<td>3.337905</td>
<td>-0.423649</td>
</tr>
<tr>
<td>H</td>
<td>2.606922</td>
<td>3.863581</td>
<td>1.856185</td>
</tr>
<tr>
<td>H</td>
<td>-0.038137</td>
<td>4.590107</td>
<td>0.578961</td>
</tr>
<tr>
<td>H</td>
<td>3.219141</td>
<td>5.780140</td>
<td>0.918387</td>
</tr>
<tr>
<td>H</td>
<td>0.687432</td>
<td>5.783449</td>
<td>2.441801</td>
</tr>
<tr>
<td>H</td>
<td>1.265107</td>
<td>2.023697</td>
<td>-5.839525</td>
</tr>
<tr>
<td>H</td>
<td>0.248026</td>
<td>1.492902</td>
<td>-4.478701</td>
</tr>
<tr>
<td>H</td>
<td>1.124726</td>
<td>0.289229</td>
<td>-5.452427</td>
</tr>
<tr>
<td>H</td>
<td>4.332453</td>
<td>1.901453</td>
<td>-5.666336</td>
</tr>
<tr>
<td>H</td>
<td>2.101217</td>
<td>3.390131</td>
<td>-2.315641</td>
</tr>
<tr>
<td>H</td>
<td>4.273247</td>
<td>0.160489</td>
<td>-5.288133</td>
</tr>
<tr>
<td>H</td>
<td>5.147605</td>
<td>1.276545</td>
<td>-4.211371</td>
</tr>
</tbody>
</table>
Table S42: B1LYP 6-311+g* TS3 coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.535348</td>
<td>4.160832</td>
<td>1.429111</td>
</tr>
<tr>
<td>C</td>
<td>0.057710</td>
<td>2.741093</td>
<td>1.608173</td>
</tr>
<tr>
<td>C</td>
<td>0.555688</td>
<td>1.729065</td>
<td>0.710520</td>
</tr>
<tr>
<td>C</td>
<td>1.650404</td>
<td>2.008983</td>
<td>-0.093285</td>
</tr>
<tr>
<td>C</td>
<td>2.269015</td>
<td>3.359197</td>
<td>-0.203282</td>
</tr>
<tr>
<td>C</td>
<td>2.009501</td>
<td>4.216352</td>
<td>1.034978</td>
</tr>
<tr>
<td>C</td>
<td>-0.030295</td>
<td>0.404107</td>
<td>0.733233</td>
</tr>
<tr>
<td>C</td>
<td>-0.986663</td>
<td>0.101208</td>
<td>1.740644</td>
</tr>
<tr>
<td>C</td>
<td>-1.394148</td>
<td>1.108036</td>
<td>2.667965</td>
</tr>
<tr>
<td>C</td>
<td>-0.872264</td>
<td>2.421832</td>
<td>2.560694</td>
</tr>
<tr>
<td>C</td>
<td>-1.550900</td>
<td>-1.203048</td>
<td>1.827588</td>
</tr>
<tr>
<td>C</td>
<td>-1.170826</td>
<td>-2.205594</td>
<td>0.895730</td>
</tr>
<tr>
<td>C</td>
<td>-0.230273</td>
<td>-1.862676</td>
<td>-0.120844</td>
</tr>
<tr>
<td>C</td>
<td>0.321181</td>
<td>-0.613564</td>
<td>-0.201564</td>
</tr>
<tr>
<td>C</td>
<td>-2.497480</td>
<td>-1.508974</td>
<td>2.846086</td>
</tr>
<tr>
<td>C</td>
<td>-3.034680</td>
<td>-2.804174</td>
<td>2.915709</td>
</tr>
<tr>
<td>C</td>
<td>-2.655520</td>
<td>-3.783493</td>
<td>2.000103</td>
</tr>
<tr>
<td>C</td>
<td>-1.736270</td>
<td>-3.489653</td>
<td>0.999038</td>
</tr>
<tr>
<td>C</td>
<td>-2.345318</td>
<td>0.777954</td>
<td>3.676341</td>
</tr>
<tr>
<td>C</td>
<td>-2.872180</td>
<td>-0.479463</td>
<td>3.764768</td>
</tr>
<tr>
<td>O</td>
<td>1.560648</td>
<td>3.760631</td>
<td>-1.348941</td>
</tr>
<tr>
<td>O</td>
<td>2.315532</td>
<td>5.595470</td>
<td>0.835109</td>
</tr>
<tr>
<td>O</td>
<td>0.288058</td>
<td>4.910796</td>
<td>2.610875</td>
</tr>
<tr>
<td>O</td>
<td>2.719854</td>
<td>3.106045</td>
<td>-3.374800</td>
</tr>
<tr>
<td>As</td>
<td>2.675570</td>
<td>1.454915</td>
<td>-3.895839</td>
</tr>
<tr>
<td>O</td>
<td>2.555866</td>
<td>0.356333</td>
<td>-2.635522</td>
</tr>
<tr>
<td>C</td>
<td>1.175998</td>
<td>1.288451</td>
<td>-5.120812</td>
</tr>
<tr>
<td>C</td>
<td>4.309001</td>
<td>1.229622</td>
<td>-4.916449</td>
</tr>
<tr>
<td>H</td>
<td>-1.224990</td>
<td>3.184118</td>
<td>-2.419777</td>
</tr>
<tr>
<td>H</td>
<td>1.017522</td>
<td>-0.398958</td>
<td>-1.002800</td>
</tr>
<tr>
<td>H</td>
<td>0.046025</td>
<td>-2.617106</td>
<td>-0.848873</td>
</tr>
<tr>
<td>H</td>
<td>-1.447239</td>
<td>-4.253782</td>
<td>0.286625</td>
</tr>
<tr>
<td>H</td>
<td>-3.080536</td>
<td>-4.777268</td>
<td>2.067594</td>
</tr>
<tr>
<td>H</td>
<td>-3.753489</td>
<td>-3.038191</td>
<td>3.692501</td>
</tr>
<tr>
<td>H</td>
<td>-3.593104</td>
<td>-0.711363</td>
<td>4.540463</td>
</tr>
<tr>
<td>H</td>
<td>-2.647768</td>
<td>1.546457</td>
<td>4.377395</td>
</tr>
<tr>
<td>H</td>
<td>2.046981</td>
<td>1.268850</td>
<td>-0.780893</td>
</tr>
<tr>
<td>H</td>
<td>3.348879</td>
<td>3.299024</td>
<td>-0.38175</td>
</tr>
<tr>
<td>H</td>
<td>2.608040</td>
<td>3.820065</td>
<td>1.863467</td>
</tr>
<tr>
<td>H</td>
<td>-0.035573</td>
<td>4.594895</td>
<td>0.597614</td>
</tr>
<tr>
<td>H</td>
<td>3.261198</td>
<td>5.740148</td>
<td>0.945333</td>
</tr>
<tr>
<td>H</td>
<td>0.677294</td>
<td>5.783858</td>
<td>2.474821</td>
</tr>
<tr>
<td>H</td>
<td>1.268879</td>
<td>2.027934</td>
<td>-5.915326</td>
</tr>
<tr>
<td>H</td>
<td>0.254646</td>
<td>1.458018</td>
<td>-4.565116</td>
</tr>
<tr>
<td>H</td>
<td>1.168088</td>
<td>0.285639</td>
<td>-5.546691</td>
</tr>
<tr>
<td>H</td>
<td>4.347060</td>
<td>1.972896</td>
<td>-5.711802</td>
</tr>
<tr>
<td>H</td>
<td>2.144398</td>
<td>3.396215</td>
<td>-2.382995</td>
</tr>
<tr>
<td>H</td>
<td>4.331366</td>
<td>0.228087</td>
<td>-5.344323</td>
</tr>
<tr>
<td>H</td>
<td>5.156639</td>
<td>1.362416</td>
<td>-4.245807</td>
</tr>
</tbody>
</table>
Table S43: B3LYP 6-311g* **TS3** coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.531248</td>
<td>4.168748</td>
<td>1.417050</td>
</tr>
<tr>
<td>C</td>
<td>0.066919</td>
<td>2.746698</td>
<td>1.597113</td>
</tr>
<tr>
<td>C</td>
<td>0.556374</td>
<td>1.744605</td>
<td>0.690787</td>
</tr>
<tr>
<td>C</td>
<td>1.659808</td>
<td>2.029672</td>
<td>-0.114415</td>
</tr>
<tr>
<td>C</td>
<td>2.277127</td>
<td>3.374933</td>
<td>-0.199200</td>
</tr>
<tr>
<td>C</td>
<td>2.004208</td>
<td>4.243423</td>
<td>1.021720</td>
</tr>
<tr>
<td>C</td>
<td>-0.027478</td>
<td>0.423658</td>
<td>0.704113</td>
</tr>
<tr>
<td>C</td>
<td>-0.974259</td>
<td>0.109987</td>
<td>1.719839</td>
</tr>
<tr>
<td>C</td>
<td>-1.371409</td>
<td>1.106904</td>
<td>2.663326</td>
</tr>
<tr>
<td>C</td>
<td>-0.853491</td>
<td>2.419661</td>
<td>2.560157</td>
</tr>
<tr>
<td>C</td>
<td>-1.537141</td>
<td>-1.195450</td>
<td>1.798818</td>
</tr>
<tr>
<td>C</td>
<td>-1.168173</td>
<td>-2.188027</td>
<td>0.849887</td>
</tr>
<tr>
<td>C</td>
<td>-0.239719</td>
<td>-1.832785</td>
<td>-0.174667</td>
</tr>
<tr>
<td>C</td>
<td>0.311944</td>
<td>-0.584090</td>
<td>-0.248828</td>
</tr>
<tr>
<td>C</td>
<td>-2.472420</td>
<td>-1.513251</td>
<td>2.825649</td>
</tr>
<tr>
<td>C</td>
<td>-3.008789</td>
<td>-2.809346</td>
<td>2.885989</td>
</tr>
<tr>
<td>C</td>
<td>-2.640681</td>
<td>-3.777159</td>
<td>1.954307</td>
</tr>
<tr>
<td>C</td>
<td>-1.733223</td>
<td>-3.472287</td>
<td>0.945445</td>
</tr>
<tr>
<td>C</td>
<td>-2.310987</td>
<td>0.763823</td>
<td>3.679922</td>
</tr>
<tr>
<td>C</td>
<td>-2.836080</td>
<td>-0.494049</td>
<td>3.760749</td>
</tr>
<tr>
<td>O</td>
<td>1.505150</td>
<td>3.715656</td>
<td>-1.334143</td>
</tr>
<tr>
<td>O</td>
<td>2.276242</td>
<td>5.624764</td>
<td>0.796710</td>
</tr>
<tr>
<td>O</td>
<td>0.284769</td>
<td>4.923098</td>
<td>2.592539</td>
</tr>
<tr>
<td>O</td>
<td>2.757391</td>
<td>3.082159</td>
<td>-3.907903</td>
</tr>
<tr>
<td>As</td>
<td>2.672979</td>
<td>1.438664</td>
<td>-3.811579</td>
</tr>
<tr>
<td>O</td>
<td>2.547783</td>
<td>0.340667</td>
<td>-2.553613</td>
</tr>
<tr>
<td>C</td>
<td>1.161133</td>
<td>1.285626</td>
<td>-5.029892</td>
</tr>
<tr>
<td>C</td>
<td>4.282722</td>
<td>1.153892</td>
<td>-4.863824</td>
</tr>
<tr>
<td>H</td>
<td>-1.196862</td>
<td>3.180564</td>
<td>3.249774</td>
</tr>
<tr>
<td>H</td>
<td>0.997448</td>
<td>-0.357959</td>
<td>-1.059323</td>
</tr>
<tr>
<td>H</td>
<td>0.025093</td>
<td>-2.579974</td>
<td>-0.916141</td>
</tr>
<tr>
<td>H</td>
<td>-1.453122</td>
<td>-4.228951</td>
<td>0.219908</td>
</tr>
<tr>
<td>H</td>
<td>-3.065758</td>
<td>-4.772631</td>
<td>2.015063</td>
</tr>
<tr>
<td>H</td>
<td>-3.719156</td>
<td>-3.052471</td>
<td>3.669279</td>
</tr>
<tr>
<td>H</td>
<td>-3.548266</td>
<td>-0.735926</td>
<td>4.543019</td>
</tr>
<tr>
<td>H</td>
<td>-2.605103</td>
<td>1.525785</td>
<td>4.393427</td>
</tr>
<tr>
<td>H</td>
<td>2.066069</td>
<td>1.291065</td>
<td>-0.803624</td>
</tr>
<tr>
<td>H</td>
<td>3.349129</td>
<td>3.346290</td>
<td>-0.424446</td>
</tr>
<tr>
<td>H</td>
<td>2.606119</td>
<td>3.867349</td>
<td>1.858882</td>
</tr>
<tr>
<td>H</td>
<td>-0.039461</td>
<td>4.591368</td>
<td>0.576719</td>
</tr>
<tr>
<td>H</td>
<td>3.216012</td>
<td>5.788880</td>
<td>0.932557</td>
</tr>
<tr>
<td>H</td>
<td>0.690008</td>
<td>5.787397</td>
<td>2.439577</td>
</tr>
<tr>
<td>H</td>
<td>1.262340</td>
<td>2.012599</td>
<td>-5.836244</td>
</tr>
<tr>
<td>H</td>
<td>0.245560</td>
<td>1.484290</td>
<td>-4.472001</td>
</tr>
<tr>
<td>H</td>
<td>1.123427</td>
<td>0.277408</td>
<td>-5.443802</td>
</tr>
<tr>
<td>H</td>
<td>4.329280</td>
<td>1.888455</td>
<td>-5.668072</td>
</tr>
<tr>
<td>H</td>
<td>2.094191</td>
<td>3.393551</td>
<td>-2.306004</td>
</tr>
<tr>
<td>H</td>
<td>4.269416</td>
<td>0.147300</td>
<td>-5.282731</td>
</tr>
<tr>
<td>H</td>
<td>5.148562</td>
<td>1.267713</td>
<td>-4.211552</td>
</tr>
</tbody>
</table>
Table S44: B3LYP 6-311+g* **TS3** coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.536087</td>
<td>4.164159</td>
<td>1.432566</td>
</tr>
<tr>
<td>C</td>
<td>0.060615</td>
<td>2.744242</td>
<td>1.610379</td>
</tr>
<tr>
<td>C</td>
<td>0.556045</td>
<td>1.735190</td>
<td>0.708799</td>
</tr>
<tr>
<td>C</td>
<td>1.652065</td>
<td>2.016273</td>
<td>-0.095858</td>
</tr>
<tr>
<td>C</td>
<td>2.271372</td>
<td>3.365063</td>
<td>-0.199580</td>
</tr>
<tr>
<td>C</td>
<td>2.010203</td>
<td>4.223484</td>
<td>1.036682</td>
</tr>
<tr>
<td>C</td>
<td>-0.031069</td>
<td>0.410871</td>
<td>0.728139</td>
</tr>
<tr>
<td>C</td>
<td>-0.985045</td>
<td>0.104484</td>
<td>1.738072</td>
</tr>
<tr>
<td>C</td>
<td>-1.388980</td>
<td>1.108266</td>
<td>2.671323</td>
</tr>
<tr>
<td>C</td>
<td>-0.866803</td>
<td>2.421936</td>
<td>2.566056</td>
</tr>
<tr>
<td>C</td>
<td>-1.549994</td>
<td>-1.199567</td>
<td>1.821345</td>
</tr>
<tr>
<td>C</td>
<td>-1.173783</td>
<td>-2.199138</td>
<td>0.883266</td>
</tr>
<tr>
<td>C</td>
<td>-0.236487</td>
<td>-1.852943</td>
<td>-0.134794</td>
</tr>
<tr>
<td>C</td>
<td>0.316415</td>
<td>-0.603134</td>
<td>-0.211791</td>
</tr>
<tr>
<td>C</td>
<td>-2.493928</td>
<td>-1.509291</td>
<td>2.842401</td>
</tr>
<tr>
<td>C</td>
<td>-3.032154</td>
<td>-2.805044</td>
<td>2.908058</td>
</tr>
<tr>
<td>C</td>
<td>-2.656853</td>
<td>-3.780823</td>
<td>1.986599</td>
</tr>
<tr>
<td>C</td>
<td>-1.740474</td>
<td>-3.483534</td>
<td>0.983272</td>
</tr>
<tr>
<td>C</td>
<td>-2.336676</td>
<td>0.774513</td>
<td>3.681448</td>
</tr>
<tr>
<td>C</td>
<td>-2.864560</td>
<td>-0.483825</td>
<td>3.766653</td>
</tr>
<tr>
<td>O</td>
<td>1.551552</td>
<td>3.758062</td>
<td>-1.344657</td>
</tr>
<tr>
<td>O</td>
<td>2.311382</td>
<td>5.604323</td>
<td>0.833738</td>
</tr>
<tr>
<td>O</td>
<td>0.288404</td>
<td>4.915254</td>
<td>2.614384</td>
</tr>
<tr>
<td>O</td>
<td>2.709566</td>
<td>3.101663</td>
<td>-3.372919</td>
</tr>
<tr>
<td>As</td>
<td>2.675529</td>
<td>1.446335</td>
<td>-3.885630</td>
</tr>
<tr>
<td>O</td>
<td>2.565932</td>
<td>0.349586</td>
<td>-2.620574</td>
</tr>
<tr>
<td>C</td>
<td>1.174086</td>
<td>1.262046</td>
<td>-5.109091</td>
</tr>
<tr>
<td>C</td>
<td>4.308565</td>
<td>1.225216</td>
<td>-4.911576</td>
</tr>
<tr>
<td>H</td>
<td>-1.217025</td>
<td>3.183666</td>
<td>3.251249</td>
</tr>
<tr>
<td>H</td>
<td>0.101616</td>
<td>-0.385559</td>
<td>-1.015215</td>
</tr>
<tr>
<td>H</td>
<td>0.036805</td>
<td>-2.605312</td>
<td>-0.867830</td>
</tr>
<tr>
<td>H</td>
<td>-1.454268</td>
<td>-4.245624</td>
<td>0.265791</td>
</tr>
<tr>
<td>H</td>
<td>-3.082998</td>
<td>-4.775562</td>
<td>2.051279</td>
</tr>
<tr>
<td>H</td>
<td>-3.749281</td>
<td>-3.041959</td>
<td>3.687143</td>
</tr>
<tr>
<td>H</td>
<td>-3.583645</td>
<td>-0.718754</td>
<td>4.544763</td>
</tr>
<tr>
<td>H</td>
<td>-2.636645</td>
<td>1.541070</td>
<td>4.387534</td>
</tr>
<tr>
<td>H</td>
<td>2.049502</td>
<td>1.276588</td>
<td>-0.786113</td>
</tr>
<tr>
<td>H</td>
<td>3.350980</td>
<td>3.310668</td>
<td>-0.391674</td>
</tr>
<tr>
<td>H</td>
<td>2.611459</td>
<td>3.829443</td>
<td>1.865750</td>
</tr>
<tr>
<td>H</td>
<td>-0.036105</td>
<td>4.597863</td>
<td>0.599753</td>
</tr>
<tr>
<td>H</td>
<td>3.256535</td>
<td>5.753896</td>
<td>0.955828</td>
</tr>
<tr>
<td>H</td>
<td>0.681246</td>
<td>5.788448</td>
<td>2.476080</td>
</tr>
<tr>
<td>H</td>
<td>1.260474</td>
<td>1.998769</td>
<td>-5.908183</td>
</tr>
<tr>
<td>H</td>
<td>0.251789</td>
<td>1.427785</td>
<td>-4.552015</td>
</tr>
<tr>
<td>H</td>
<td>1.173442</td>
<td>0.256017</td>
<td>-5.529802</td>
</tr>
<tr>
<td>H</td>
<td>4.338790</td>
<td>1.964529</td>
<td>-5.712225</td>
</tr>
<tr>
<td>H</td>
<td>2.129375</td>
<td>3.394335</td>
<td>-2.370351</td>
</tr>
<tr>
<td>H</td>
<td>4.335852</td>
<td>0.220269</td>
<td>-5.33518</td>
</tr>
<tr>
<td>H</td>
<td>5.157963</td>
<td>1.367992</td>
<td>-4.243735</td>
</tr>
</tbody>
</table>
Table S45: BPW91 6-311g* BPDE coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.741332</td>
<td>0.782002</td>
<td>-0.163064</td>
</tr>
<tr>
<td>C</td>
<td>-0.669341</td>
<td>1.673722</td>
<td>-0.148745</td>
</tr>
<tr>
<td>C</td>
<td>0.662042</td>
<td>1.198808</td>
<td>-0.064202</td>
</tr>
<tr>
<td>C</td>
<td>0.914455</td>
<td>-0.201645</td>
<td>-0.029772</td>
</tr>
<tr>
<td>C</td>
<td>2.239598</td>
<td>-0.768014</td>
<td>0.014313</td>
</tr>
<tr>
<td>C</td>
<td>2.446364</td>
<td>-2.121009</td>
<td>0.057754</td>
</tr>
<tr>
<td>C</td>
<td>1.352882</td>
<td>-3.050555</td>
<td>0.065309</td>
</tr>
<tr>
<td>C</td>
<td>1.545865</td>
<td>-4.446493</td>
<td>0.116862</td>
</tr>
<tr>
<td>C</td>
<td>0.452472</td>
<td>-5.318059</td>
<td>0.117290</td>
</tr>
<tr>
<td>C</td>
<td>-0.852887</td>
<td>-4.819899</td>
<td>0.064162</td>
</tr>
<tr>
<td>C</td>
<td>-1.095752</td>
<td>-3.431168</td>
<td>0.009392</td>
</tr>
<tr>
<td>C</td>
<td>-2.425056</td>
<td>-2.888089</td>
<td>-0.048639</td>
</tr>
<tr>
<td>C</td>
<td>-2.635180</td>
<td>-1.536286</td>
<td>-0.102201</td>
</tr>
<tr>
<td>C</td>
<td>-1.536784</td>
<td>-0.609572</td>
<td>-0.100903</td>
</tr>
<tr>
<td>C</td>
<td>-0.197825</td>
<td>-1.114520</td>
<td>-0.039738</td>
</tr>
<tr>
<td>C</td>
<td>0.019806</td>
<td>-2.527336</td>
<td>0.011347</td>
</tr>
<tr>
<td>C</td>
<td>1.768232</td>
<td>2.192351</td>
<td>0.038820</td>
</tr>
<tr>
<td>C</td>
<td>1.472922</td>
<td>3.601940</td>
<td>0.374985</td>
</tr>
<tr>
<td>C</td>
<td>0.036101</td>
<td>3.995890</td>
<td>0.604304</td>
</tr>
<tr>
<td>C</td>
<td>-0.918297</td>
<td>3.162596</td>
<td>-0.271253</td>
</tr>
<tr>
<td>O</td>
<td>1.837947</td>
<td>3.245506</td>
<td>-0.982379</td>
</tr>
<tr>
<td>O</td>
<td>-0.221481</td>
<td>5.397782</td>
<td>0.397461</td>
</tr>
<tr>
<td>O</td>
<td>-2.272196</td>
<td>3.476521</td>
<td>0.059887</td>
</tr>
<tr>
<td>H</td>
<td>-2.757356</td>
<td>1.174623</td>
<td>-0.216765</td>
</tr>
<tr>
<td>H</td>
<td>3.110026</td>
<td>-0.112579</td>
<td>-0.003193</td>
</tr>
<tr>
<td>H</td>
<td>3.465902</td>
<td>-2.513544</td>
<td>0.083634</td>
</tr>
<tr>
<td>H</td>
<td>2.563407</td>
<td>-4.842435</td>
<td>0.156296</td>
</tr>
<tr>
<td>H</td>
<td>0.619072</td>
<td>-6.396502</td>
<td>0.158516</td>
</tr>
<tr>
<td>H</td>
<td>-1.701518</td>
<td>-5.508195</td>
<td>0.064287</td>
</tr>
<tr>
<td>H</td>
<td>-3.272205</td>
<td>-3.578354</td>
<td>-0.050250</td>
</tr>
<tr>
<td>H</td>
<td>-3.651398</td>
<td>-1.137209</td>
<td>-0.147817</td>
</tr>
<tr>
<td>H</td>
<td>2.755756</td>
<td>1.825009</td>
<td>0.319743</td>
</tr>
<tr>
<td>H</td>
<td>2.230228</td>
<td>4.185939</td>
<td>0.090275</td>
</tr>
<tr>
<td>H</td>
<td>-0.241661</td>
<td>3.821817</td>
<td>1.662990</td>
</tr>
<tr>
<td>H</td>
<td>-0.719618</td>
<td>3.451711</td>
<td>-1.329317</td>
</tr>
<tr>
<td>H</td>
<td>0.085440</td>
<td>5.626005</td>
<td>-0.493346</td>
</tr>
<tr>
<td>H</td>
<td>-2.305456</td>
<td>4.451854</td>
<td>0.074952</td>
</tr>
</tbody>
</table>
Table S46: BPW91 6-311+g* BPDE coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.744336</td>
<td>0.780231</td>
<td>-0.149142</td>
</tr>
<tr>
<td>C</td>
<td>-0.673186</td>
<td>1.674199</td>
<td>-0.129131</td>
</tr>
<tr>
<td>C</td>
<td>0.657803</td>
<td>1.198584</td>
<td>-0.043362</td>
</tr>
<tr>
<td>C</td>
<td>0.911933</td>
<td>-0.202196</td>
<td>-0.016014</td>
</tr>
<tr>
<td>C</td>
<td>2.237898</td>
<td>-0.767039</td>
<td>0.024693</td>
</tr>
<tr>
<td>C</td>
<td>2.446065</td>
<td>-2.120622</td>
<td>0.061251</td>
</tr>
<tr>
<td>C</td>
<td>1.353311</td>
<td>-3.051237</td>
<td>0.064344</td>
</tr>
<tr>
<td>C</td>
<td>1.547967</td>
<td>-4.447561</td>
<td>0.108332</td>
</tr>
<tr>
<td>C</td>
<td>0.455090</td>
<td>-5.320447</td>
<td>0.103169</td>
</tr>
<tr>
<td>C</td>
<td>-0.851124</td>
<td>-4.822871</td>
<td>0.051650</td>
</tr>
<tr>
<td>C</td>
<td>-1.094873</td>
<td>-3.433750</td>
<td>0.004220</td>
</tr>
<tr>
<td>C</td>
<td>-2.424819</td>
<td>-2.891470</td>
<td>-0.052659</td>
</tr>
<tr>
<td>C</td>
<td>-2.636124</td>
<td>-1.539117</td>
<td>-0.100062</td>
</tr>
<tr>
<td>C</td>
<td>-1.537936</td>
<td>-0.611605</td>
<td>-0.092071</td>
</tr>
<tr>
<td>C</td>
<td>-0.198976</td>
<td>-1.115973</td>
<td>-0.031199</td>
</tr>
<tr>
<td>C</td>
<td>0.019852</td>
<td>-2.529082</td>
<td>0.012353</td>
</tr>
<tr>
<td>C</td>
<td>1.766425</td>
<td>2.187304</td>
<td>0.057410</td>
</tr>
<tr>
<td>C</td>
<td>1.477827</td>
<td>3.602005</td>
<td>0.370971</td>
</tr>
<tr>
<td>C</td>
<td>0.044251</td>
<td>4.012517</td>
<td>0.589721</td>
</tr>
<tr>
<td>C</td>
<td>-0.924958</td>
<td>3.164198</td>
<td>-0.255822</td>
</tr>
<tr>
<td>O</td>
<td>1.853057</td>
<td>3.228068</td>
<td>-0.980087</td>
</tr>
<tr>
<td>O</td>
<td>-0.193917</td>
<td>5.413921</td>
<td>0.346776</td>
</tr>
<tr>
<td>O</td>
<td>-2.279664</td>
<td>3.470369</td>
<td>0.096770</td>
</tr>
<tr>
<td>H</td>
<td>-2.761831</td>
<td>1.168816</td>
<td>-0.204771</td>
</tr>
<tr>
<td>H</td>
<td>3.108140</td>
<td>-0.111138</td>
<td>0.010563</td>
</tr>
<tr>
<td>H</td>
<td>3.466270</td>
<td>-2.512062</td>
<td>0.084645</td>
</tr>
<tr>
<td>H</td>
<td>2.566005</td>
<td>-4.842906</td>
<td>0.146079</td>
</tr>
<tr>
<td>H</td>
<td>0.622627</td>
<td>-6.399130</td>
<td>0.138438</td>
</tr>
<tr>
<td>H</td>
<td>-1.699203</td>
<td>-5.512129</td>
<td>0.047044</td>
</tr>
<tr>
<td>H</td>
<td>-3.271678</td>
<td>-3.582334</td>
<td>-0.059119</td>
</tr>
<tr>
<td>H</td>
<td>-3.652921</td>
<td>-1.141051</td>
<td>-0.145326</td>
</tr>
<tr>
<td>H</td>
<td>2.749437</td>
<td>1.819555</td>
<td>0.352623</td>
</tr>
<tr>
<td>H</td>
<td>2.235789</td>
<td>4.186007</td>
<td>0.904285</td>
</tr>
<tr>
<td>H</td>
<td>-0.197416</td>
<td>3.873215</td>
<td>1.655520</td>
</tr>
<tr>
<td>H</td>
<td>-0.759211</td>
<td>3.443820</td>
<td>-1.315256</td>
</tr>
<tr>
<td>H</td>
<td>0.124100</td>
<td>5.630278</td>
<td>-0.549935</td>
</tr>
<tr>
<td>H</td>
<td>-2.351505</td>
<td>4.443338</td>
<td>0.063276</td>
</tr>
</tbody>
</table>
Table S47: BLYP 6-311g* BPDE coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.746417</td>
<td>0.781985</td>
<td>-0.155433</td>
</tr>
<tr>
<td>C</td>
<td>-0.672748</td>
<td>1.676827</td>
<td>-0.138534</td>
</tr>
<tr>
<td>C</td>
<td>0.663199</td>
<td>1.201098</td>
<td>-0.054440</td>
</tr>
<tr>
<td>C</td>
<td>0.917309</td>
<td>-0.203721</td>
<td>-0.022360</td>
</tr>
<tr>
<td>C</td>
<td>2.246588</td>
<td>-0.773453</td>
<td>0.022045</td>
</tr>
<tr>
<td>C</td>
<td>2.453494</td>
<td>-2.128991</td>
<td>0.062272</td>
</tr>
<tr>
<td>C</td>
<td>1.357502</td>
<td>-3.062566</td>
<td>0.065553</td>
</tr>
<tr>
<td>C</td>
<td>1.550100</td>
<td>-4.462372</td>
<td>0.113049</td>
</tr>
<tr>
<td>C</td>
<td>0.454133</td>
<td>-5.336052</td>
<td>0.109318</td>
</tr>
<tr>
<td>C</td>
<td>-0.854538</td>
<td>-4.837129</td>
<td>0.056168</td>
</tr>
<tr>
<td>C</td>
<td>-1.099196</td>
<td>-3.444914</td>
<td>0.005525</td>
</tr>
<tr>
<td>C</td>
<td>-2.432223</td>
<td>-2.898677</td>
<td>-0.052552</td>
</tr>
<tr>
<td>C</td>
<td>-2.642844</td>
<td>-1.544346</td>
<td>-0.102058</td>
</tr>
<tr>
<td>C</td>
<td>-1.541858</td>
<td>-0.613337</td>
<td>-0.096678</td>
</tr>
<tr>
<td>C</td>
<td>-0.198589</td>
<td>-1.120103</td>
<td>-0.035560</td>
</tr>
<tr>
<td>C</td>
<td>0.019964</td>
<td>-2.537657</td>
<td>0.011637</td>
</tr>
<tr>
<td>C</td>
<td>1.774530</td>
<td>2.197853</td>
<td>0.049688</td>
</tr>
<tr>
<td>C</td>
<td>1.482711</td>
<td>3.615195</td>
<td>0.376139</td>
</tr>
<tr>
<td>C</td>
<td>0.041352</td>
<td>4.018585</td>
<td>0.593686</td>
</tr>
<tr>
<td>C</td>
<td>-0.924798</td>
<td>3.173674</td>
<td>-0.265039</td>
</tr>
<tr>
<td>O</td>
<td>1.853537</td>
<td>3.254376</td>
<td>-0.991251</td>
</tr>
<tr>
<td>O</td>
<td>-0.207696</td>
<td>5.430274</td>
<td>0.371188</td>
</tr>
<tr>
<td>O</td>
<td>-2.286495</td>
<td>3.486359</td>
<td>0.085849</td>
</tr>
<tr>
<td>H</td>
<td>-2.762121</td>
<td>1.173600</td>
<td>-0.209774</td>
</tr>
<tr>
<td>H</td>
<td>3.116478</td>
<td>-0.118199</td>
<td>0.007862</td>
</tr>
<tr>
<td>H</td>
<td>3.472889</td>
<td>-2.521419</td>
<td>0.089112</td>
</tr>
<tr>
<td>H</td>
<td>2.567129</td>
<td>-4.859104</td>
<td>0.152501</td>
</tr>
<tr>
<td>H</td>
<td>0.620921</td>
<td>-6.414438</td>
<td>0.147206</td>
</tr>
<tr>
<td>H</td>
<td>-1.702263</td>
<td>-5.526241</td>
<td>0.053045</td>
</tr>
<tr>
<td>H</td>
<td>-3.279364</td>
<td>-3.588677</td>
<td>-0.057467</td>
</tr>
<tr>
<td>H</td>
<td>-3.658983</td>
<td>-1.145530</td>
<td>-0.147588</td>
</tr>
<tr>
<td>H</td>
<td>2.760601</td>
<td>1.829299</td>
<td>0.329823</td>
</tr>
<tr>
<td>H</td>
<td>2.238154</td>
<td>4.203828</td>
<td>0.907239</td>
</tr>
<tr>
<td>H</td>
<td>-0.210872</td>
<td>3.866725</td>
<td>1.660470</td>
</tr>
<tr>
<td>H</td>
<td>-0.746489</td>
<td>3.461335</td>
<td>-1.319301</td>
</tr>
<tr>
<td>H</td>
<td>0.099619</td>
<td>5.645277</td>
<td>-0.531837</td>
</tr>
<tr>
<td>H</td>
<td>-2.332550</td>
<td>4.463340</td>
<td>0.074993</td>
</tr>
</tbody>
</table>
Table S48: BLYP 6-311+g* BPDE coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.749712</td>
<td>0.780283</td>
<td>-0.139396</td>
</tr>
<tr>
<td>C</td>
<td>-0.677080</td>
<td>1.677980</td>
<td>-0.114637</td>
</tr>
<tr>
<td>C</td>
<td>0.658498</td>
<td>1.201198</td>
<td>-0.029408</td>
</tr>
<tr>
<td>C</td>
<td>0.914517</td>
<td>-0.204242</td>
<td>-0.006148</td>
</tr>
<tr>
<td>C</td>
<td>2.244823</td>
<td>-0.772259</td>
<td>0.034610</td>
</tr>
<tr>
<td>C</td>
<td>2.453368</td>
<td>-2.128657</td>
<td>0.066529</td>
</tr>
<tr>
<td>C</td>
<td>1.358111</td>
<td>-3.063406</td>
<td>0.064004</td>
</tr>
<tr>
<td>C</td>
<td>1.552709</td>
<td>-4.463760</td>
<td>0.102623</td>
</tr>
<tr>
<td>C</td>
<td>0.457178</td>
<td>-5.338984</td>
<td>0.092475</td>
</tr>
<tr>
<td>C</td>
<td>-0.852624</td>
<td>-4.840611</td>
<td>0.041272</td>
</tr>
<tr>
<td>C</td>
<td>-1.098151</td>
<td>-3.447816</td>
<td>-0.000834</td>
</tr>
<tr>
<td>C</td>
<td>-2.431993</td>
<td>-2.902463</td>
<td>-0.057615</td>
</tr>
<tr>
<td>C</td>
<td>-2.643939</td>
<td>-1.547315</td>
<td>-0.099928</td>
</tr>
<tr>
<td>C</td>
<td>-1.543024</td>
<td>-0.615454</td>
<td>-0.086712</td>
</tr>
<tr>
<td>C</td>
<td>-0.199771</td>
<td>-1.121652</td>
<td>-0.025849</td>
</tr>
<tr>
<td>C</td>
<td>0.020119</td>
<td>-2.539644</td>
<td>0.012475</td>
</tr>
<tr>
<td>C</td>
<td>1.772441</td>
<td>2.191827</td>
<td>0.073051</td>
</tr>
<tr>
<td>C</td>
<td>1.489013</td>
<td>3.614775</td>
<td>0.371632</td>
</tr>
<tr>
<td>C</td>
<td>0.051812</td>
<td>4.038249</td>
<td>0.581507</td>
</tr>
<tr>
<td>C</td>
<td>-0.933153</td>
<td>3.176224</td>
<td>-0.245566</td>
</tr>
<tr>
<td>O</td>
<td>1.872782</td>
<td>3.233408</td>
<td>-0.989030</td>
</tr>
<tr>
<td>O</td>
<td>-0.173185</td>
<td>5.449148</td>
<td>0.309434</td>
</tr>
<tr>
<td>O</td>
<td>-2.294870</td>
<td>3.479702</td>
<td>0.136102</td>
</tr>
<tr>
<td>H</td>
<td>-2.766990</td>
<td>1.16963</td>
<td>-0.196471</td>
</tr>
<tr>
<td>H</td>
<td>3.114494</td>
<td>-0.116782</td>
<td>0.025574</td>
</tr>
<tr>
<td>H</td>
<td>3.473362</td>
<td>-2.519646</td>
<td>0.090714</td>
</tr>
<tr>
<td>H</td>
<td>2.570100</td>
<td>-4.859742</td>
<td>0.140067</td>
</tr>
<tr>
<td>H</td>
<td>0.624963</td>
<td>-6.417420</td>
<td>0.123482</td>
</tr>
<tr>
<td>H</td>
<td>-1.699590</td>
<td>-5.530608</td>
<td>0.032771</td>
</tr>
<tr>
<td>H</td>
<td>-3.278715</td>
<td>-3.592889</td>
<td>-0.068080</td>
</tr>
<tr>
<td>H</td>
<td>-3.660567</td>
<td>-1.149806</td>
<td>-0.145047</td>
</tr>
<tr>
<td>H</td>
<td>2.753188</td>
<td>1.822924</td>
<td>0.369411</td>
</tr>
<tr>
<td>H</td>
<td>2.245256</td>
<td>4.203213</td>
<td>0.901203</td>
</tr>
<tr>
<td>H</td>
<td>-0.189403</td>
<td>3.928348</td>
<td>1.649962</td>
</tr>
<tr>
<td>H</td>
<td>-0.797798</td>
<td>3.452424</td>
<td>-1.308084</td>
</tr>
<tr>
<td>H</td>
<td>0.146472</td>
<td>5.649240</td>
<td>-0.593571</td>
</tr>
<tr>
<td>H</td>
<td>-2.392474</td>
<td>4.449955</td>
<td>0.057656</td>
</tr>
</tbody>
</table>
Table S49: B1LYP 6-311g* BPDE coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.733016</td>
<td>0.776024</td>
<td>-0.154713</td>
</tr>
<tr>
<td>C</td>
<td>-0.666335</td>
<td>1.663859</td>
<td>-0.137112</td>
</tr>
<tr>
<td>C</td>
<td>0.657226</td>
<td>1.189831</td>
<td>-0.055949</td>
</tr>
<tr>
<td>C</td>
<td>0.908197</td>
<td>-0.201385</td>
<td>-0.020669</td>
</tr>
<tr>
<td>C</td>
<td>2.233469</td>
<td>-0.768334</td>
<td>0.027396</td>
</tr>
<tr>
<td>C</td>
<td>2.437783</td>
<td>-2.110026</td>
<td>0.068297</td>
</tr>
<tr>
<td>C</td>
<td>1.345069</td>
<td>-3.039771</td>
<td>0.068500</td>
</tr>
<tr>
<td>C</td>
<td>1.538272</td>
<td>-4.427556</td>
<td>0.115692</td>
</tr>
<tr>
<td>C</td>
<td>0.450437</td>
<td>-5.295576</td>
<td>0.109329</td>
</tr>
<tr>
<td>C</td>
<td>-0.848620</td>
<td>-4.799594</td>
<td>0.054058</td>
</tr>
<tr>
<td>C</td>
<td>-1.088956</td>
<td>-3.418547</td>
<td>0.004062</td>
</tr>
<tr>
<td>C</td>
<td>-2.417551</td>
<td>-2.875148</td>
<td>-0.056071</td>
</tr>
<tr>
<td>C</td>
<td>-2.625927</td>
<td>-1.534620</td>
<td>-0.105130</td>
</tr>
<tr>
<td>C</td>
<td>-1.528082</td>
<td>-0.607585</td>
<td>-0.097669</td>
</tr>
<tr>
<td>C</td>
<td>-0.197405</td>
<td>-1.109386</td>
<td>-0.035160</td>
</tr>
<tr>
<td>C</td>
<td>0.019936</td>
<td>-2.520148</td>
<td>0.012409</td>
</tr>
<tr>
<td>C</td>
<td>1.764326</td>
<td>2.184183</td>
<td>0.037537</td>
</tr>
<tr>
<td>C</td>
<td>1.472928</td>
<td>3.585909</td>
<td>0.367732</td>
</tr>
<tr>
<td>C</td>
<td>0.041988</td>
<td>3.987181</td>
<td>0.596644</td>
</tr>
<tr>
<td>C</td>
<td>-0.918794</td>
<td>3.151728</td>
<td>-0.258767</td>
</tr>
<tr>
<td>O</td>
<td>1.824831</td>
<td>3.222300</td>
<td>-0.979320</td>
</tr>
<tr>
<td>O</td>
<td>-0.197186</td>
<td>5.378551</td>
<td>0.368118</td>
</tr>
<tr>
<td>O</td>
<td>-2.261527</td>
<td>3.453275</td>
<td>0.096613</td>
</tr>
<tr>
<td>H</td>
<td>-2.741294</td>
<td>1.164779</td>
<td>-0.207614</td>
</tr>
<tr>
<td>H</td>
<td>3.096525</td>
<td>-0.117560</td>
<td>0.016888</td>
</tr>
<tr>
<td>H</td>
<td>3.448972</td>
<td>-2.500968</td>
<td>0.098356</td>
</tr>
<tr>
<td>H</td>
<td>2.547883</td>
<td>-4.820998</td>
<td>0.150995</td>
</tr>
<tr>
<td>H</td>
<td>0.615966</td>
<td>-6.366011</td>
<td>0.146853</td>
</tr>
<tr>
<td>H</td>
<td>-1.696039</td>
<td>-5.483246</td>
<td>0.048786</td>
</tr>
<tr>
<td>H</td>
<td>-3.257454</td>
<td>-3.561211</td>
<td>-0.062404</td>
</tr>
<tr>
<td>H</td>
<td>-3.633891</td>
<td>-1.137321</td>
<td>-0.151788</td>
</tr>
<tr>
<td>H</td>
<td>2.744778</td>
<td>1.818392</td>
<td>0.308580</td>
</tr>
<tr>
<td>H</td>
<td>2.225073</td>
<td>4.174291</td>
<td>0.885789</td>
</tr>
<tr>
<td>H</td>
<td>-0.203102</td>
<td>3.830914</td>
<td>1.650255</td>
</tr>
<tr>
<td>H</td>
<td>-0.749020</td>
<td>3.438241</td>
<td>-1.305470</td>
</tr>
<tr>
<td>H</td>
<td>0.110609</td>
<td>5.603248</td>
<td>-0.518350</td>
</tr>
<tr>
<td>H</td>
<td>-2.335544</td>
<td>4.414992</td>
<td>0.077472</td>
</tr>
</tbody>
</table>
Table S50: B1LYP 6-311+g* BPDE coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.735780</td>
<td>0.774781</td>
<td>-0.142433</td>
</tr>
<tr>
<td>C</td>
<td>-0.669759</td>
<td>1.664851</td>
<td>-0.119406</td>
</tr>
<tr>
<td>C</td>
<td>0.653489</td>
<td>1.190028</td>
<td>-0.037391</td>
</tr>
<tr>
<td>C</td>
<td>0.905972</td>
<td>-0.201710</td>
<td>-0.009130</td>
</tr>
<tr>
<td>C</td>
<td>2.232096</td>
<td>-0.767301</td>
<td>0.035426</td>
</tr>
<tr>
<td>C</td>
<td>2.437731</td>
<td>-2.109843</td>
<td>0.070073</td>
</tr>
<tr>
<td>C</td>
<td>1.345561</td>
<td>-3.040459</td>
<td>0.066758</td>
</tr>
<tr>
<td>C</td>
<td>1.540408</td>
<td>-4.428744</td>
<td>0.107637</td>
</tr>
<tr>
<td>C</td>
<td>0.452847</td>
<td>-5.298063</td>
<td>0.097123</td>
</tr>
<tr>
<td>C</td>
<td>-0.847210</td>
<td>-4.802455</td>
<td>0.043640</td>
</tr>
<tr>
<td>C</td>
<td>-1.088221</td>
<td>-3.420880</td>
<td>-0.000328</td>
</tr>
<tr>
<td>C</td>
<td>-2.417499</td>
<td>-2.878244</td>
<td>-0.059134</td>
</tr>
<tr>
<td>C</td>
<td>-2.626954</td>
<td>-1.536921</td>
<td>-0.103039</td>
</tr>
<tr>
<td>C</td>
<td>-1.529146</td>
<td>-0.609218</td>
<td>-0.090061</td>
</tr>
<tr>
<td>C</td>
<td>-0.198401</td>
<td>-1.110588</td>
<td>-0.028285</td>
</tr>
<tr>
<td>C</td>
<td>0.020010</td>
<td>-2.521709</td>
<td>0.012824</td>
</tr>
<tr>
<td>C</td>
<td>1.762989</td>
<td>2.179503</td>
<td>0.055534</td>
</tr>
<tr>
<td>C</td>
<td>1.477973</td>
<td>3.585680</td>
<td>0.365121</td>
</tr>
<tr>
<td>C</td>
<td>0.049911</td>
<td>4.002428</td>
<td>0.583744</td>
</tr>
<tr>
<td>C</td>
<td>-0.925178</td>
<td>3.153871</td>
<td>-0.244411</td>
</tr>
<tr>
<td>O</td>
<td>1.840634</td>
<td>3.206296</td>
<td>-0.976272</td>
</tr>
<tr>
<td>O</td>
<td>-0.171571</td>
<td>5.392856</td>
<td>0.323549</td>
</tr>
<tr>
<td>O</td>
<td>-2.267367</td>
<td>3.448849</td>
<td>0.131754</td>
</tr>
<tr>
<td>H</td>
<td>-2.745364</td>
<td>1.159726</td>
<td>-0.197001</td>
</tr>
<tr>
<td>H</td>
<td>3.095055</td>
<td>-0.116411</td>
<td>0.027845</td>
</tr>
<tr>
<td>H</td>
<td>3.449458</td>
<td>-2.499665</td>
<td>0.097402</td>
</tr>
<tr>
<td>H</td>
<td>2.550350</td>
<td>-4.821633</td>
<td>0.147136</td>
</tr>
<tr>
<td>H</td>
<td>0.619174</td>
<td>-6.368555</td>
<td>0.129761</td>
</tr>
<tr>
<td>H</td>
<td>-1.688405</td>
<td>-5.486847</td>
<td>0.034870</td>
</tr>
<tr>
<td>H</td>
<td>-3.257128</td>
<td>-3.564645</td>
<td>-0.069237</td>
</tr>
<tr>
<td>H</td>
<td>-3.635395</td>
<td>-1.140716</td>
<td>-0.149062</td>
</tr>
<tr>
<td>H</td>
<td>2.738840</td>
<td>1.812772</td>
<td>0.340580</td>
</tr>
<tr>
<td>H</td>
<td>2.230686</td>
<td>4.173122</td>
<td>0.883147</td>
</tr>
<tr>
<td>H</td>
<td>-0.186402</td>
<td>3.877132</td>
<td>1.643256</td>
</tr>
<tr>
<td>H</td>
<td>-0.785469</td>
<td>3.431408</td>
<td>-1.297302</td>
</tr>
<tr>
<td>H</td>
<td>0.145146</td>
<td>5.609761</td>
<td>-0.562580</td>
</tr>
<tr>
<td>H</td>
<td>-2.382911</td>
<td>4.404247</td>
<td>0.058066</td>
</tr>
</tbody>
</table>
Table S51: B3LYP 6-311g* BPDE coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.73364</td>
<td>0.776538</td>
<td>-0.155644</td>
</tr>
<tr>
<td>C</td>
<td>-0.666568</td>
<td>1.664563</td>
<td>-0.138635</td>
</tr>
<tr>
<td>C</td>
<td>0.657737</td>
<td>1.190638</td>
<td>-0.057073</td>
</tr>
<tr>
<td>C</td>
<td>0.908912</td>
<td>-0.201505</td>
<td>-0.021953</td>
</tr>
<tr>
<td>C</td>
<td>2.233346</td>
<td>-0.767991</td>
<td>0.025625</td>
</tr>
<tr>
<td>C</td>
<td>2.438024</td>
<td>-2.111042</td>
<td>0.066872</td>
</tr>
<tr>
<td>C</td>
<td>1.345904</td>
<td>-3.040262</td>
<td>0.068014</td>
</tr>
<tr>
<td>C</td>
<td>1.538859</td>
<td>-4.428809</td>
<td>0.115768</td>
</tr>
<tr>
<td>C</td>
<td>0.450639</td>
<td>-5.297025</td>
<td>0.110307</td>
</tr>
<tr>
<td>C</td>
<td>-0.848871</td>
<td>-4.800982</td>
<td>0.055351</td>
</tr>
<tr>
<td>C</td>
<td>-1.089718</td>
<td>-3.419309</td>
<td>0.004729</td>
</tr>
<tr>
<td>C</td>
<td>-2.417600</td>
<td>-2.876221</td>
<td>-0.055044</td>
</tr>
<tr>
<td>C</td>
<td>-2.626230</td>
<td>-1.534336</td>
<td>-0.104651</td>
</tr>
<tr>
<td>C</td>
<td>-1.529045</td>
<td>-0.607808</td>
<td>-0.098050</td>
</tr>
<tr>
<td>C</td>
<td>-0.197426</td>
<td>-1.109997</td>
<td>-0.035806</td>
</tr>
<tr>
<td>C</td>
<td>0.019878</td>
<td>-2.520266</td>
<td>0.012202</td>
</tr>
<tr>
<td>C</td>
<td>1.764230</td>
<td>2.184303</td>
<td>0.037703</td>
</tr>
<tr>
<td>C</td>
<td>1.472464</td>
<td>3.587026</td>
<td>0.368585</td>
</tr>
<tr>
<td>C</td>
<td>0.041266</td>
<td>3.987123</td>
<td>0.597211</td>
</tr>
<tr>
<td>C</td>
<td>-0.918549</td>
<td>3.151889</td>
<td>-0.260262</td>
</tr>
<tr>
<td>C</td>
<td>1.826705</td>
<td>3.224658</td>
<td>-0.979682</td>
</tr>
<tr>
<td>C</td>
<td>-0.200773</td>
<td>5.379585</td>
<td>0.371564</td>
</tr>
<tr>
<td>C</td>
<td>-2.262499</td>
<td>3.455522</td>
<td>0.091673</td>
</tr>
<tr>
<td>H</td>
<td>-2.742908</td>
<td>1.166149</td>
<td>-0.208465</td>
</tr>
<tr>
<td>H</td>
<td>3.097410</td>
<td>-0.16507</td>
<td>0.014219</td>
</tr>
<tr>
<td>H</td>
<td>3.450396</td>
<td>-2.502151</td>
<td>0.096456</td>
</tr>
<tr>
<td>H</td>
<td>2.549576</td>
<td>-4.822577</td>
<td>0.156820</td>
</tr>
<tr>
<td>H</td>
<td>0.616338</td>
<td>-6.368554</td>
<td>0.148321</td>
</tr>
<tr>
<td>H</td>
<td>-1.691560</td>
<td>-5.485322</td>
<td>0.050805</td>
</tr>
<tr>
<td>H</td>
<td>-3.258537</td>
<td>-3.562839</td>
<td>-0.060744</td>
</tr>
<tr>
<td>H</td>
<td>-3.635378</td>
<td>-1.36873</td>
<td>-0.151114</td>
</tr>
<tr>
<td>H</td>
<td>2.745557</td>
<td>1.818205</td>
<td>0.310576</td>
</tr>
<tr>
<td>H</td>
<td>2.225122</td>
<td>4.174663</td>
<td>0.889418</td>
</tr>
<tr>
<td>H</td>
<td>-0.204691</td>
<td>3.828466</td>
<td>1.651577</td>
</tr>
<tr>
<td>H</td>
<td>-0.744656</td>
<td>3.438853</td>
<td>-1.307751</td>
</tr>
<tr>
<td>H</td>
<td>0.106837</td>
<td>5.605145</td>
<td>-0.516714</td>
</tr>
<tr>
<td>H</td>
<td>-2.330382</td>
<td>4.419752</td>
<td>0.077969</td>
</tr>
</tbody>
</table>
Table S52: B3LYP 6-311+g* BPDE coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-1.749712</td>
<td>0.780283</td>
<td>-0.139396</td>
</tr>
<tr>
<td>C</td>
<td>-0.677080</td>
<td>1.677980</td>
<td>-0.114637</td>
</tr>
<tr>
<td>C</td>
<td>0.658498</td>
<td>1.201198</td>
<td>-0.029408</td>
</tr>
<tr>
<td>C</td>
<td>0.914517</td>
<td>-0.204242</td>
<td>-0.006148</td>
</tr>
<tr>
<td>C</td>
<td>2.244823</td>
<td>-0.772259</td>
<td>0.034610</td>
</tr>
<tr>
<td>C</td>
<td>2.453368</td>
<td>-2.128657</td>
<td>0.066529</td>
</tr>
<tr>
<td>C</td>
<td>1.358111</td>
<td>-3.063406</td>
<td>0.064004</td>
</tr>
<tr>
<td>C</td>
<td>1.552709</td>
<td>-4.463760</td>
<td>0.102623</td>
</tr>
<tr>
<td>C</td>
<td>0.457178</td>
<td>-5.338984</td>
<td>0.092475</td>
</tr>
<tr>
<td>C</td>
<td>-0.852624</td>
<td>-4.840611</td>
<td>0.041272</td>
</tr>
<tr>
<td>C</td>
<td>-1.098151</td>
<td>-3.447816</td>
<td>-0.000834</td>
</tr>
<tr>
<td>C</td>
<td>-2.431993</td>
<td>-2.902463</td>
<td>-0.057615</td>
</tr>
<tr>
<td>C</td>
<td>-2.643939</td>
<td>-1.547315</td>
<td>-0.099928</td>
</tr>
<tr>
<td>C</td>
<td>-1.543024</td>
<td>-0.615454</td>
<td>-0.086712</td>
</tr>
<tr>
<td>C</td>
<td>-0.199771</td>
<td>-1.121652</td>
<td>-0.025849</td>
</tr>
<tr>
<td>C</td>
<td>0.020119</td>
<td>-2.539644</td>
<td>0.012475</td>
</tr>
<tr>
<td>C</td>
<td>1.772441</td>
<td>2.191827</td>
<td>0.073051</td>
</tr>
<tr>
<td>C</td>
<td>1.489013</td>
<td>3.614775</td>
<td>0.371632</td>
</tr>
<tr>
<td>C</td>
<td>0.051812</td>
<td>4.038249</td>
<td>0.581507</td>
</tr>
<tr>
<td>C</td>
<td>-0.933153</td>
<td>3.176224</td>
<td>-0.245566</td>
</tr>
<tr>
<td>O</td>
<td>1.872782</td>
<td>3.233408</td>
<td>-0.989030</td>
</tr>
<tr>
<td>O</td>
<td>-0.173185</td>
<td>5.449148</td>
<td>0.309434</td>
</tr>
<tr>
<td>O</td>
<td>-2.294870</td>
<td>3.479702</td>
<td>0.136102</td>
</tr>
<tr>
<td>H</td>
<td>-2.766990</td>
<td>1.166963</td>
<td>-0.196471</td>
</tr>
<tr>
<td>H</td>
<td>3.114494</td>
<td>-0.116782</td>
<td>0.025574</td>
</tr>
<tr>
<td>H</td>
<td>3.473362</td>
<td>-2.519646</td>
<td>0.090714</td>
</tr>
<tr>
<td>H</td>
<td>2.570100</td>
<td>-4.859742</td>
<td>0.140067</td>
</tr>
<tr>
<td>H</td>
<td>0.624963</td>
<td>-6.417420</td>
<td>0.123482</td>
</tr>
<tr>
<td>H</td>
<td>-1.699590</td>
<td>-5.530608</td>
<td>0.032771</td>
</tr>
<tr>
<td>H</td>
<td>-3.278715</td>
<td>-3.592889</td>
<td>-0.068080</td>
</tr>
<tr>
<td>H</td>
<td>-3.660567</td>
<td>-1.149806</td>
<td>-0.145047</td>
</tr>
<tr>
<td>H</td>
<td>2.753188</td>
<td>1.822924</td>
<td>0.369411</td>
</tr>
<tr>
<td>H</td>
<td>2.245256</td>
<td>4.203213</td>
<td>0.901203</td>
</tr>
<tr>
<td>H</td>
<td>-0.189403</td>
<td>3.928348</td>
<td>1.649962</td>
</tr>
<tr>
<td>H</td>
<td>-0.797798</td>
<td>3.452424</td>
<td>-1.308084</td>
</tr>
<tr>
<td>H</td>
<td>0.146472</td>
<td>5.649240</td>
<td>-0.593571</td>
</tr>
<tr>
<td>H</td>
<td>-2.392474</td>
<td>4.449955</td>
<td>0.057656</td>
</tr>
</tbody>
</table>
Table S53: BPW91 6-311g* Tetrol coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>12.422420</td>
<td>0.761389</td>
<td>1.400775</td>
</tr>
<tr>
<td>C</td>
<td>11.881851</td>
<td>-0.427734</td>
<td>1.897763</td>
</tr>
<tr>
<td>C</td>
<td>12.717584</td>
<td>-1.467784</td>
<td>2.319099</td>
</tr>
<tr>
<td>C</td>
<td>14.120220</td>
<td>-1.338771</td>
<td>2.254392</td>
</tr>
<tr>
<td>C</td>
<td>15.007792</td>
<td>-2.389132</td>
<td>2.676545</td>
</tr>
<tr>
<td>C</td>
<td>16.366458</td>
<td>-2.240218</td>
<td>2.605867</td>
</tr>
<tr>
<td>C</td>
<td>16.959516</td>
<td>-1.026557</td>
<td>2.110730</td>
</tr>
<tr>
<td>C</td>
<td>18.350770</td>
<td>-0.848090</td>
<td>2.047212</td>
</tr>
<tr>
<td>C</td>
<td>18.918684</td>
<td>0.343126</td>
<td>1.576021</td>
</tr>
<tr>
<td>C</td>
<td>20.426334</td>
<td>0.491908</td>
<td>1.633985</td>
</tr>
<tr>
<td>C</td>
<td>20.955321</td>
<td>1.525513</td>
<td>0.645103</td>
</tr>
<tr>
<td>C</td>
<td>20.199503</td>
<td>2.847242</td>
<td>0.789195</td>
</tr>
<tr>
<td>C</td>
<td>18.691668</td>
<td>2.671486</td>
<td>0.541550</td>
</tr>
<tr>
<td>C</td>
<td>18.097069</td>
<td>1.398501</td>
<td>1.125503</td>
</tr>
<tr>
<td>C</td>
<td>16.678942</td>
<td>1.253253</td>
<td>1.173659</td>
</tr>
<tr>
<td>C</td>
<td>15.778337</td>
<td>2.286812</td>
<td>0.730998</td>
</tr>
<tr>
<td>C</td>
<td>14.418286</td>
<td>2.136988</td>
<td>0.804769</td>
</tr>
<tr>
<td>C</td>
<td>13.820105</td>
<td>0.937097</td>
<td>1.316859</td>
</tr>
<tr>
<td>C</td>
<td>14.685304</td>
<td>-0.119749</td>
<td>1.749755</td>
</tr>
<tr>
<td>C</td>
<td>16.104820</td>
<td>0.039247</td>
<td>1.677327</td>
</tr>
<tr>
<td>O</td>
<td>21.054522</td>
<td>-0.779003</td>
<td>1.419689</td>
</tr>
<tr>
<td>O</td>
<td>22.349753</td>
<td>1.694129</td>
<td>0.981646</td>
</tr>
<tr>
<td>O</td>
<td>20.379942</td>
<td>3.375386</td>
<td>2.110592</td>
</tr>
<tr>
<td>H</td>
<td>11.763117</td>
<td>1.567725</td>
<td>1.070726</td>
</tr>
<tr>
<td>H</td>
<td>10.797958</td>
<td>-0.547388</td>
<td>1.956573</td>
</tr>
<tr>
<td>H</td>
<td>12.285599</td>
<td>-2.394783</td>
<td>2.703985</td>
</tr>
<tr>
<td>H</td>
<td>14.573973</td>
<td>-3.316674</td>
<td>3.058220</td>
</tr>
<tr>
<td>H</td>
<td>17.027924</td>
<td>-3.047062</td>
<td>2.931052</td>
</tr>
<tr>
<td>H</td>
<td>19.011391</td>
<td>-1.651143</td>
<td>2.377206</td>
</tr>
<tr>
<td>H</td>
<td>20.685671</td>
<td>0.859776</td>
<td>2.646146</td>
</tr>
<tr>
<td>H</td>
<td>20.852250</td>
<td>1.132585</td>
<td>-0.381168</td>
</tr>
<tr>
<td>H</td>
<td>20.568449</td>
<td>3.568010</td>
<td>0.036003</td>
</tr>
<tr>
<td>H</td>
<td>18.205173</td>
<td>3.553040</td>
<td>0.987160</td>
</tr>
<tr>
<td>H</td>
<td>16.189064</td>
<td>3.199155</td>
<td>0.301122</td>
</tr>
<tr>
<td>H</td>
<td>13.763044</td>
<td>2.942563</td>
<td>0.463654</td>
</tr>
<tr>
<td>H</td>
<td>22.011221</td>
<td>-0.595918</td>
<td>1.457842</td>
</tr>
<tr>
<td>H</td>
<td>22.807823</td>
<td>2.071090</td>
<td>0.211099</td>
</tr>
<tr>
<td>O</td>
<td>18.413405</td>
<td>2.770710</td>
<td>-0.875928</td>
</tr>
<tr>
<td>H</td>
<td>18.481483</td>
<td>1.876662</td>
<td>-1.254556</td>
</tr>
<tr>
<td>H</td>
<td>21.335113</td>
<td>3.289931</td>
<td>2.294678</td>
</tr>
</tbody>
</table>
Table S54: BPW91 6-311+g* Tertol coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>12.421511</td>
<td>0.768684</td>
<td>1.412878</td>
</tr>
<tr>
<td>C</td>
<td>11.881192</td>
<td>-0.420772</td>
<td>1.910530</td>
</tr>
<tr>
<td>C</td>
<td>12.717887</td>
<td>-1.461884</td>
<td>2.328841</td>
</tr>
<tr>
<td>C</td>
<td>14.120670</td>
<td>-1.335352</td>
<td>2.259789</td>
</tr>
<tr>
<td>C</td>
<td>15.008328</td>
<td>-2.384483</td>
<td>2.680651</td>
</tr>
<tr>
<td>C</td>
<td>16.367344</td>
<td>-2.236777</td>
<td>2.605948</td>
</tr>
<tr>
<td>C</td>
<td>16.959533</td>
<td>-1.024457</td>
<td>2.105688</td>
</tr>
<tr>
<td>C</td>
<td>18.351232</td>
<td>-0.848699</td>
<td>2.038035</td>
</tr>
<tr>
<td>C</td>
<td>18.921102</td>
<td>0.337057</td>
<td>1.554451</td>
</tr>
<tr>
<td>C</td>
<td>20.432175</td>
<td>0.477027</td>
<td>1.606950</td>
</tr>
<tr>
<td>C</td>
<td>20.969018</td>
<td>1.546185</td>
<td>0.659461</td>
</tr>
<tr>
<td>C</td>
<td>20.189070</td>
<td>2.854190</td>
<td>0.806897</td>
</tr>
<tr>
<td>C</td>
<td>18.695133</td>
<td>2.653728</td>
<td>0.504024</td>
</tr>
<tr>
<td>C</td>
<td>18.098278</td>
<td>1.392398</td>
<td>1.104525</td>
</tr>
<tr>
<td>C</td>
<td>16.679396</td>
<td>1.254563</td>
<td>1.167108</td>
</tr>
<tr>
<td>C</td>
<td>15.777434</td>
<td>2.292131</td>
<td>0.736639</td>
</tr>
<tr>
<td>C</td>
<td>14.416960</td>
<td>2.144692</td>
<td>0.816933</td>
</tr>
<tr>
<td>C</td>
<td>13.819435</td>
<td>0.942713</td>
<td>1.324641</td>
</tr>
<tr>
<td>C</td>
<td>14.685291</td>
<td>-0.115345</td>
<td>1.752733</td>
</tr>
<tr>
<td>C</td>
<td>16.104957</td>
<td>0.041642</td>
<td>1.673639</td>
</tr>
<tr>
<td>O</td>
<td>21.045154</td>
<td>-0.796289</td>
<td>1.336323</td>
</tr>
<tr>
<td>O</td>
<td>22.357095</td>
<td>1.727121</td>
<td>1.019489</td>
</tr>
<tr>
<td>O</td>
<td>20.301530</td>
<td>3.372435</td>
<td>2.142113</td>
</tr>
<tr>
<td>H</td>
<td>11.761825</td>
<td>1.576457</td>
<td>1.086562</td>
</tr>
<tr>
<td>H</td>
<td>10.797234</td>
<td>-0.530652</td>
<td>1.972631</td>
</tr>
<tr>
<td>H</td>
<td>12.286322</td>
<td>-2.388799</td>
<td>2.714899</td>
</tr>
<tr>
<td>H</td>
<td>14.574882</td>
<td>-3.31297</td>
<td>3.064960</td>
</tr>
<tr>
<td>H</td>
<td>17.028886</td>
<td>-3.043929</td>
<td>2.930672</td>
</tr>
<tr>
<td>H</td>
<td>19.008592</td>
<td>-1.651958</td>
<td>2.374260</td>
</tr>
<tr>
<td>H</td>
<td>20.704288</td>
<td>0.786870</td>
<td>2.634477</td>
</tr>
<tr>
<td>H</td>
<td>20.895117</td>
<td>1.183117</td>
<td>-0.380079</td>
</tr>
<tr>
<td>H</td>
<td>20.574377</td>
<td>3.594324</td>
<td>0.082481</td>
</tr>
<tr>
<td>H</td>
<td>18.181722</td>
<td>3.543872</td>
<td>0.897239</td>
</tr>
<tr>
<td>H</td>
<td>16.182243</td>
<td>3.215271</td>
<td>0.323049</td>
</tr>
<tr>
<td>H</td>
<td>13.761872</td>
<td>2.954489</td>
<td>0.485226</td>
</tr>
<tr>
<td>H</td>
<td>22.006722</td>
<td>-0.654342</td>
<td>1.417858</td>
</tr>
<tr>
<td>H</td>
<td>22.833467</td>
<td>2.104672</td>
<td>0.259405</td>
</tr>
<tr>
<td>O</td>
<td>18.477976</td>
<td>2.702182</td>
<td>-0.930554</td>
</tr>
<tr>
<td>H</td>
<td>18.511127</td>
<td>1.792045</td>
<td>-1.276326</td>
</tr>
<tr>
<td>H</td>
<td>21.251481</td>
<td>3.357668</td>
<td>2.367803</td>
</tr>
</tbody>
</table>
Table S55: BLYP 6-311g* Tetrrol coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>12.404382</td>
<td>0.758633</td>
<td>1.404444</td>
</tr>
<tr>
<td>C</td>
<td>11.863802</td>
<td>-0.431886</td>
<td>1.907311</td>
</tr>
<tr>
<td>C</td>
<td>12.702313</td>
<td>-1.473451</td>
<td>2.330798</td>
</tr>
<tr>
<td>C</td>
<td>14.108393</td>
<td>-1.345332</td>
<td>2.262649</td>
</tr>
<tr>
<td>C</td>
<td>15.000762</td>
<td>-2.397286</td>
<td>2.686986</td>
</tr>
<tr>
<td>C</td>
<td>16.361512</td>
<td>-2.248275</td>
<td>2.613035</td>
</tr>
<tr>
<td>C</td>
<td>16.956895</td>
<td>-1.032521</td>
<td>2.111759</td>
</tr>
<tr>
<td>C</td>
<td>18.351174</td>
<td>-0.853957</td>
<td>2.044714</td>
</tr>
<tr>
<td>C</td>
<td>18.920987</td>
<td>0.338611</td>
<td>1.569168</td>
</tr>
<tr>
<td>C</td>
<td>20.437306</td>
<td>0.485194</td>
<td>1.627310</td>
</tr>
<tr>
<td>C</td>
<td>20.973703</td>
<td>1.532513</td>
<td>0.646649</td>
</tr>
<tr>
<td>C</td>
<td>20.211657</td>
<td>2.858460</td>
<td>0.789956</td>
</tr>
<tr>
<td>C</td>
<td>18.696869</td>
<td>2.680491</td>
<td>0.541672</td>
</tr>
<tr>
<td>C</td>
<td>18.097199</td>
<td>1.397571</td>
<td>1.117745</td>
</tr>
<tr>
<td>C</td>
<td>16.674192</td>
<td>1.252653</td>
<td>1.165988</td>
</tr>
<tr>
<td>C</td>
<td>15.767717</td>
<td>2.287111</td>
<td>0.719783</td>
</tr>
<tr>
<td>C</td>
<td>14.405510</td>
<td>2.136511</td>
<td>0.796972</td>
</tr>
<tr>
<td>C</td>
<td>13.805352</td>
<td>0.935341</td>
<td>1.316235</td>
</tr>
<tr>
<td>C</td>
<td>14.674606</td>
<td>-0.123674</td>
<td>1.751555</td>
</tr>
<tr>
<td>C</td>
<td>16.098708</td>
<td>0.035762</td>
<td>1.675472</td>
</tr>
<tr>
<td>O</td>
<td>21.063011</td>
<td>-0.796529</td>
<td>1.389165</td>
</tr>
<tr>
<td>O</td>
<td>22.376447</td>
<td>1.703885</td>
<td>0.996963</td>
</tr>
<tr>
<td>O</td>
<td>20.386395</td>
<td>3.390092</td>
<td>2.123022</td>
</tr>
<tr>
<td>H</td>
<td>11.743798</td>
<td>1.563415</td>
<td>1.073739</td>
</tr>
<tr>
<td>H</td>
<td>10.780176</td>
<td>-0.551230</td>
<td>1.968951</td>
</tr>
<tr>
<td>H</td>
<td>12.270264</td>
<td>-2.398734</td>
<td>2.719182</td>
</tr>
<tr>
<td>H</td>
<td>14.567913</td>
<td>-3.323677</td>
<td>3.072078</td>
</tr>
<tr>
<td>H</td>
<td>17.023461</td>
<td>-3.054125</td>
<td>2.939119</td>
</tr>
<tr>
<td>H</td>
<td>19.011329</td>
<td>-1.656710</td>
<td>2.374448</td>
</tr>
<tr>
<td>H</td>
<td>20.704613</td>
<td>0.831066</td>
<td>2.643392</td>
</tr>
<tr>
<td>H</td>
<td>20.883810</td>
<td>1.147321</td>
<td>-0.382686</td>
</tr>
<tr>
<td>H</td>
<td>20.582007</td>
<td>3.582591</td>
<td>0.042619</td>
</tr>
<tr>
<td>H</td>
<td>18.208663</td>
<td>3.559688</td>
<td>0.986588</td>
</tr>
<tr>
<td>H</td>
<td>16.176263</td>
<td>3.195810</td>
<td>0.282328</td>
</tr>
<tr>
<td>H</td>
<td>13.749795</td>
<td>2.940398</td>
<td>0.453259</td>
</tr>
<tr>
<td>H</td>
<td>22.023474</td>
<td>-0.623764</td>
<td>1.440457</td>
</tr>
<tr>
<td>H</td>
<td>22.841830</td>
<td>2.082834</td>
<td>0.228343</td>
</tr>
<tr>
<td>O</td>
<td>18.421032</td>
<td>2.795298</td>
<td>-0.888809</td>
</tr>
<tr>
<td>H</td>
<td>18.486137</td>
<td>1.903310</td>
<td>-1.279608</td>
</tr>
<tr>
<td>H</td>
<td>21.344401</td>
<td>3.319103</td>
<td>2.310100</td>
</tr>
</tbody>
</table>
Table S56: BLYP 6-311+g* Tetrol coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>12.403012</td>
<td>0.764988</td>
<td>1.415947</td>
</tr>
<tr>
<td>C</td>
<td>11.863053</td>
<td>-0.426493</td>
<td>1.919039</td>
</tr>
<tr>
<td>C</td>
<td>12.703129</td>
<td>-1.468407</td>
<td>2.340850</td>
</tr>
<tr>
<td>C</td>
<td>14.109485</td>
<td>-1.339579</td>
<td>2.269807</td>
</tr>
<tr>
<td>C</td>
<td>15.002364</td>
<td>-2.391066</td>
<td>2.694891</td>
</tr>
<tr>
<td>C</td>
<td>16.363672</td>
<td>-2.242119</td>
<td>2.618215</td>
</tr>
<tr>
<td>C</td>
<td>16.957568</td>
<td>-1.027921</td>
<td>2.110170</td>
</tr>
<tr>
<td>C</td>
<td>18.352414</td>
<td>-0.851921</td>
<td>2.038350</td>
</tr>
<tr>
<td>C</td>
<td>18.924261</td>
<td>0.333211</td>
<td>1.545289</td>
</tr>
<tr>
<td>C</td>
<td>20.444097</td>
<td>0.467893</td>
<td>1.593273</td>
</tr>
<tr>
<td>C</td>
<td>20.989931</td>
<td>1.558754</td>
<td>0.664042</td>
</tr>
<tr>
<td>C</td>
<td>20.197984</td>
<td>2.867593</td>
<td>0.809930</td>
</tr>
<tr>
<td>C</td>
<td>18.700330</td>
<td>2.659429</td>
<td>0.495389</td>
</tr>
<tr>
<td>C</td>
<td>18.098482</td>
<td>1.391425</td>
<td>1.093440</td>
</tr>
<tr>
<td>C</td>
<td>16.674604</td>
<td>1.255345</td>
<td>1.160425</td>
</tr>
<tr>
<td>C</td>
<td>15.766157</td>
<td>2.294285</td>
<td>0.728501</td>
</tr>
<tr>
<td>C</td>
<td>14.403323</td>
<td>2.145444</td>
<td>0.811879</td>
</tr>
<tr>
<td>C</td>
<td>13.804355</td>
<td>0.940981</td>
<td>1.324788</td>
</tr>
<tr>
<td>C</td>
<td>14.674750</td>
<td>-0.118572</td>
<td>1.756058</td>
</tr>
<tr>
<td>C</td>
<td>16.099091</td>
<td>0.039671</td>
<td>1.673712</td>
</tr>
<tr>
<td>O</td>
<td>21.050524</td>
<td>-0.815654</td>
<td>1.280941</td>
</tr>
<tr>
<td>O</td>
<td>22.384361</td>
<td>1.747105</td>
<td>1.045072</td>
</tr>
<tr>
<td>O</td>
<td>20.291640</td>
<td>3.387898</td>
<td>2.159621</td>
</tr>
<tr>
<td>H</td>
<td>11.741859</td>
<td>1.570593</td>
<td>1.088474</td>
</tr>
<tr>
<td>H</td>
<td>10.779591</td>
<td>-0.545085</td>
<td>1.982734</td>
</tr>
<tr>
<td>H</td>
<td>12.271986</td>
<td>-2.393689</td>
<td>2.730210</td>
</tr>
<tr>
<td>H</td>
<td>14.570450</td>
<td>-3.316550</td>
<td>3.083101</td>
</tr>
<tr>
<td>H</td>
<td>17.025795</td>
<td>-3.047339</td>
<td>2.945307</td>
</tr>
<tr>
<td>H</td>
<td>19.008636</td>
<td>-1.653983</td>
<td>2.377369</td>
</tr>
<tr>
<td>H</td>
<td>20.730287</td>
<td>0.740076</td>
<td>2.625642</td>
</tr>
<tr>
<td>H</td>
<td>20.937134</td>
<td>1.209379</td>
<td>-0.379921</td>
</tr>
<tr>
<td>H</td>
<td>20.587346</td>
<td>3.615100</td>
<td>0.097942</td>
</tr>
<tr>
<td>H</td>
<td>18.179655</td>
<td>3.549088</td>
<td>0.874914</td>
</tr>
<tr>
<td>H</td>
<td>16.167254</td>
<td>3.217152</td>
<td>0.313028</td>
</tr>
<tr>
<td>H</td>
<td>13.747687</td>
<td>2.954023</td>
<td>0.479402</td>
</tr>
<tr>
<td>H</td>
<td>22.015669</td>
<td>-0.696850</td>
<td>1.384286</td>
</tr>
<tr>
<td>H</td>
<td>22.872864</td>
<td>2.123788</td>
<td>0.288739</td>
</tr>
<tr>
<td>O</td>
<td>18.499347</td>
<td>2.709990</td>
<td>-0.956650</td>
</tr>
<tr>
<td>H</td>
<td>18.521420</td>
<td>1.798436</td>
<td>-1.307153</td>
</tr>
<tr>
<td>H</td>
<td>21.241486</td>
<td>3.397804</td>
<td>2.395796</td>
</tr>
</tbody>
</table>
Table S57: B1LYP 6-311g* Tetrol coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>12.444928</td>
<td>0.755930</td>
<td>1.392443</td>
</tr>
<tr>
<td>C</td>
<td>11.907006</td>
<td>-0.425017</td>
<td>1.892668</td>
</tr>
<tr>
<td>C</td>
<td>12.739563</td>
<td>-1.456844</td>
<td>2.319710</td>
</tr>
<tr>
<td>C</td>
<td>14.133605</td>
<td>-1.326451</td>
<td>2.256642</td>
</tr>
<tr>
<td>C</td>
<td>15.021768</td>
<td>-2.372871</td>
<td>2.686758</td>
</tr>
<tr>
<td>C</td>
<td>16.368756</td>
<td>-2.224498</td>
<td>2.618002</td>
</tr>
<tr>
<td>C</td>
<td>16.962094</td>
<td>-1.013887</td>
<td>2.115844</td>
</tr>
<tr>
<td>C</td>
<td>18.344980</td>
<td>-0.838787</td>
<td>2.051094</td>
</tr>
<tr>
<td>C</td>
<td>18.910699</td>
<td>0.343757</td>
<td>1.574189</td>
</tr>
<tr>
<td>C</td>
<td>20.418463</td>
<td>0.484533</td>
<td>1.620467</td>
</tr>
<tr>
<td>C</td>
<td>20.941321</td>
<td>1.526986</td>
<td>0.644804</td>
</tr>
<tr>
<td>C</td>
<td>20.187298</td>
<td>2.841267</td>
<td>0.806944</td>
</tr>
<tr>
<td>C</td>
<td>18.686749</td>
<td>2.667881</td>
<td>0.550543</td>
</tr>
<tr>
<td>C</td>
<td>18.092487</td>
<td>1.391923</td>
<td>1.125807</td>
</tr>
<tr>
<td>C</td>
<td>16.682578</td>
<td>1.247319</td>
<td>1.171879</td>
</tr>
<tr>
<td>C</td>
<td>15.781411</td>
<td>2.277872</td>
<td>0.722585</td>
</tr>
<tr>
<td>C</td>
<td>14.432790</td>
<td>2.127522</td>
<td>0.793961</td>
</tr>
<tr>
<td>C</td>
<td>13.834903</td>
<td>0.930490</td>
<td>1.311035</td>
</tr>
<tr>
<td>C</td>
<td>14.694882</td>
<td>-0.117034</td>
<td>1.748495</td>
</tr>
<tr>
<td>C</td>
<td>16.112071</td>
<td>0.042605</td>
<td>1.677398</td>
</tr>
<tr>
<td>O</td>
<td>21.027871</td>
<td>-0.780243</td>
<td>1.372208</td>
</tr>
<tr>
<td>O</td>
<td>22.329105</td>
<td>1.691273</td>
<td>0.963934</td>
</tr>
<tr>
<td>O</td>
<td>20.351898</td>
<td>3.344812</td>
<td>2.130632</td>
</tr>
<tr>
<td>H</td>
<td>11.790105</td>
<td>1.553502</td>
<td>1.059298</td>
</tr>
<tr>
<td>H</td>
<td>10.831264</td>
<td>-0.544578</td>
<td>1.949629</td>
</tr>
<tr>
<td>H</td>
<td>12.310537</td>
<td>-2.374780</td>
<td>2.706315</td>
</tr>
<tr>
<td>H</td>
<td>14.590148</td>
<td>-3.290919</td>
<td>3.070335</td>
</tr>
<tr>
<td>H</td>
<td>17.026455</td>
<td>-3.021949</td>
<td>2.946233</td>
</tr>
<tr>
<td>H</td>
<td>18.999576</td>
<td>-1.635655</td>
<td>2.379956</td>
</tr>
<tr>
<td>H</td>
<td>20.693581</td>
<td>0.821900</td>
<td>2.627552</td>
</tr>
<tr>
<td>H</td>
<td>20.829608</td>
<td>1.149716</td>
<td>-0.376817</td>
</tr>
<tr>
<td>H</td>
<td>20.558196</td>
<td>3.570746</td>
<td>0.078049</td>
</tr>
<tr>
<td>H</td>
<td>18.201219</td>
<td>3.537402</td>
<td>0.997077</td>
</tr>
<tr>
<td>H</td>
<td>16.188957</td>
<td>3.181576</td>
<td>0.293230</td>
</tr>
<tr>
<td>H</td>
<td>13.781206</td>
<td>2.923434</td>
<td>0.449564</td>
</tr>
<tr>
<td>H</td>
<td>21.979687</td>
<td>-0.633336</td>
<td>1.420460</td>
</tr>
<tr>
<td>H</td>
<td>22.787231</td>
<td>2.069555</td>
<td>0.206554</td>
</tr>
<tr>
<td>O</td>
<td>18.422015</td>
<td>2.774996</td>
<td>-0.858568</td>
</tr>
<tr>
<td>H</td>
<td>18.465069</td>
<td>1.897182</td>
<td>-1.252598</td>
</tr>
<tr>
<td>H</td>
<td>21.295783</td>
<td>3.305994</td>
<td>2.328439</td>
</tr>
</tbody>
</table>
Table S58: B1LYP 6-311+g* Tetrol coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>12.443472</td>
<td>0.760599</td>
<td>1.402170</td>
</tr>
<tr>
<td>C</td>
<td>11.906043</td>
<td>-0.420981</td>
<td>1.903187</td>
</tr>
<tr>
<td>C</td>
<td>12.740006</td>
<td>-1.453346</td>
<td>2.328294</td>
</tr>
<tr>
<td>C</td>
<td>14.134338</td>
<td>-1.322735</td>
<td>2.261772</td>
</tr>
<tr>
<td>C</td>
<td>15.022875</td>
<td>-2.369212</td>
<td>2.691472</td>
</tr>
<tr>
<td>C</td>
<td>16.370458</td>
<td>-2.221315</td>
<td>2.619361</td>
</tr>
<tr>
<td>C</td>
<td>16.962537</td>
<td>-1.011828</td>
<td>2.112030</td>
</tr>
<tr>
<td>C</td>
<td>18.345921</td>
<td>-0.838895</td>
<td>2.042942</td>
</tr>
<tr>
<td>C</td>
<td>18.913017</td>
<td>0.338861</td>
<td>1.554461</td>
</tr>
<tr>
<td>C</td>
<td>20.423872</td>
<td>0.471825</td>
<td>1.595798</td>
</tr>
<tr>
<td>C</td>
<td>20.954300</td>
<td>1.546239</td>
<td>0.657478</td>
</tr>
<tr>
<td>C</td>
<td>20.178214</td>
<td>2.848248</td>
<td>0.822856</td>
</tr>
<tr>
<td>C</td>
<td>18.689668</td>
<td>2.653162</td>
<td>0.517425</td>
</tr>
<tr>
<td>C</td>
<td>18.093398</td>
<td>1.386969</td>
<td>1.106869</td>
</tr>
<tr>
<td>C</td>
<td>16.682752</td>
<td>1.248554</td>
<td>1.166323</td>
</tr>
<tr>
<td>C</td>
<td>15.779928</td>
<td>2.282381</td>
<td>0.727668</td>
</tr>
<tr>
<td>C</td>
<td>14.430643</td>
<td>2.133552</td>
<td>0.804475</td>
</tr>
<tr>
<td>C</td>
<td>13.833829</td>
<td>0.934257</td>
<td>1.317518</td>
</tr>
<tr>
<td>C</td>
<td>14.694840</td>
<td>-0.113857</td>
<td>1.751313</td>
</tr>
<tr>
<td>C</td>
<td>16.112261</td>
<td>0.044620</td>
<td>1.674559</td>
</tr>
<tr>
<td>O</td>
<td>21.019683</td>
<td>-0.793540</td>
<td>1.297888</td>
</tr>
<tr>
<td>O</td>
<td>22.336510</td>
<td>1.722618</td>
<td>0.998556</td>
</tr>
<tr>
<td>O</td>
<td>20.284047</td>
<td>3.342292</td>
<td>2.158358</td>
</tr>
<tr>
<td>H</td>
<td>11.788085</td>
<td>1.558928</td>
<td>1.071869</td>
</tr>
<tr>
<td>H</td>
<td>10.830407</td>
<td>-0.540370</td>
<td>1.962656</td>
</tr>
<tr>
<td>H</td>
<td>12.311739</td>
<td>-2.371173</td>
<td>2.716095</td>
</tr>
<tr>
<td>H</td>
<td>14.592027</td>
<td>-3.286533</td>
<td>3.076995</td>
</tr>
<tr>
<td>H</td>
<td>17.028315</td>
<td>-3.018643</td>
<td>2.947578</td>
</tr>
<tr>
<td>H</td>
<td>18.997679</td>
<td>-1.635536</td>
<td>2.378016</td>
</tr>
<tr>
<td>H</td>
<td>20.709194</td>
<td>0.758367</td>
<td>2.615187</td>
</tr>
<tr>
<td>H</td>
<td>20.869707</td>
<td>1.196220</td>
<td>-0.375956</td>
</tr>
<tr>
<td>H</td>
<td>20.562682</td>
<td>3.594545</td>
<td>0.119748</td>
</tr>
<tr>
<td>H</td>
<td>18.180230</td>
<td>3.530466</td>
<td>0.917663</td>
</tr>
<tr>
<td>H</td>
<td>16.181587</td>
<td>3.196209</td>
<td>0.313274</td>
</tr>
<tr>
<td>H</td>
<td>13.778993</td>
<td>2.932957</td>
<td>0.468394</td>
</tr>
<tr>
<td>H</td>
<td>21.974557</td>
<td>-0.688468</td>
<td>1.389708</td>
</tr>
<tr>
<td>H</td>
<td>22.814446</td>
<td>2.093295</td>
<td>0.248720</td>
</tr>
<tr>
<td>O</td>
<td>18.480083</td>
<td>2.715462</td>
<td>-0.907063</td>
</tr>
<tr>
<td>H</td>
<td>18.484767</td>
<td>1.824037</td>
<td>-1.273791</td>
</tr>
<tr>
<td>H</td>
<td>21.220754</td>
<td>3.375087</td>
<td>2.390286</td>
</tr>
</tbody>
</table>
Table S59: B3LYP 6-311g* Tetrol coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>12.443316</td>
<td>0.756756</td>
<td>1.394118</td>
</tr>
<tr>
<td>C</td>
<td>11.905200</td>
<td>-0.424976</td>
<td>1.893611</td>
</tr>
<tr>
<td>C</td>
<td>12.737844</td>
<td>-1.457781</td>
<td>2.319328</td>
</tr>
<tr>
<td>C</td>
<td>14.132721</td>
<td>-1.327910</td>
<td>2.255880</td>
</tr>
<tr>
<td>C</td>
<td>15.020312</td>
<td>-2.374394</td>
<td>2.684203</td>
</tr>
<tr>
<td>C</td>
<td>16.368727</td>
<td>-2.226057</td>
<td>2.615055</td>
</tr>
<tr>
<td>C</td>
<td>16.961770</td>
<td>-1.015674</td>
<td>2.114465</td>
</tr>
<tr>
<td>C</td>
<td>18.345425</td>
<td>-0.839932</td>
<td>2.049835</td>
</tr>
<tr>
<td>C</td>
<td>18.911163</td>
<td>0.343582</td>
<td>1.574387</td>
</tr>
<tr>
<td>C</td>
<td>20.418242</td>
<td>0.485764</td>
<td>1.622620</td>
</tr>
<tr>
<td>C</td>
<td>20.942060</td>
<td>1.526246</td>
<td>0.645181</td>
</tr>
<tr>
<td>C</td>
<td>20.188112</td>
<td>2.841324</td>
<td>0.804105</td>
</tr>
<tr>
<td>C</td>
<td>18.686741</td>
<td>2.667789</td>
<td>0.550184</td>
</tr>
<tr>
<td>C</td>
<td>18.092772</td>
<td>1.392504</td>
<td>1.125880</td>
</tr>
<tr>
<td>C</td>
<td>16.682101</td>
<td>1.247899</td>
<td>1.172039</td>
</tr>
<tr>
<td>C</td>
<td>15.781554</td>
<td>2.278304</td>
<td>0.724013</td>
</tr>
<tr>
<td>C</td>
<td>14.431558</td>
<td>2.128162</td>
<td>0.795925</td>
</tr>
<tr>
<td>C</td>
<td>13.839332</td>
<td>0.931467</td>
<td>1.312068</td>
</tr>
<tr>
<td>C</td>
<td>14.694481</td>
<td>-0.117328</td>
<td>1.748492</td>
</tr>
<tr>
<td>C</td>
<td>16.111223</td>
<td>0.042034</td>
<td>1.677112</td>
</tr>
<tr>
<td>O</td>
<td>21.031026</td>
<td>-0.779479</td>
<td>1.380491</td>
</tr>
<tr>
<td>O</td>
<td>22.330456</td>
<td>1.691142</td>
<td>0.967044</td>
</tr>
<tr>
<td>O</td>
<td>20.356277</td>
<td>3.349283</td>
<td>2.126564</td>
</tr>
<tr>
<td>H</td>
<td>11.787913</td>
<td>1.555675</td>
<td>1.061659</td>
</tr>
<tr>
<td>H</td>
<td>10.828345</td>
<td>-0.544435</td>
<td>1.951017</td>
</tr>
<tr>
<td>H</td>
<td>12.308409</td>
<td>-2.377012</td>
<td>2.705583</td>
</tr>
<tr>
<td>H</td>
<td>14.588424</td>
<td>-3.293844</td>
<td>3.067349</td>
</tr>
<tr>
<td>H</td>
<td>17.026874</td>
<td>-3.024975</td>
<td>2.942605</td>
</tr>
<tr>
<td>H</td>
<td>19.001088</td>
<td>-1.637659</td>
<td>2.378420</td>
</tr>
<tr>
<td>H</td>
<td>20.690744</td>
<td>0.828489</td>
<td>2.630226</td>
</tr>
<tr>
<td>H</td>
<td>20.831761</td>
<td>1.146430</td>
<td>-0.376957</td>
</tr>
<tr>
<td>H</td>
<td>20.558255</td>
<td>3.568779</td>
<td>0.070763</td>
</tr>
<tr>
<td>H</td>
<td>18.201672</td>
<td>3.538738</td>
<td>0.997844</td>
</tr>
<tr>
<td>H</td>
<td>16.189679</td>
<td>3.182877</td>
<td>0.294029</td>
</tr>
<tr>
<td>H</td>
<td>13.779488</td>
<td>2.925482</td>
<td>0.452105</td>
</tr>
<tr>
<td>H</td>
<td>21.983871</td>
<td>-0.627013</td>
<td>1.427665</td>
</tr>
<tr>
<td>H</td>
<td>22.789441</td>
<td>2.069474</td>
<td>0.208008</td>
</tr>
<tr>
<td>O</td>
<td>18.419021</td>
<td>2.775214</td>
<td>-0.859539</td>
</tr>
<tr>
<td>H</td>
<td>18.463535</td>
<td>1.895093</td>
<td>-1.252531</td>
</tr>
<tr>
<td>H</td>
<td>21.302325</td>
<td>3.303282</td>
<td>2.322002</td>
</tr>
</tbody>
</table>
Table S60: B3LYP 6-311+g* Tertol coordinates (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x (Å)</th>
<th>y (Å)</th>
<th>z (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>12.441937</td>
<td>0.761590</td>
<td>1.404154</td>
</tr>
<tr>
<td>C</td>
<td>11.904347</td>
<td>-0.420879</td>
<td>1.904137</td>
</tr>
<tr>
<td>C</td>
<td>12.738386</td>
<td>-1.454272</td>
<td>2.327675</td>
</tr>
<tr>
<td>C</td>
<td>14.133526</td>
<td>-1.324147</td>
<td>2.260853</td>
</tr>
<tr>
<td>C</td>
<td>15.021510</td>
<td>-2.370737</td>
<td>2.688545</td>
</tr>
<tr>
<td>C</td>
<td>16.370466</td>
<td>-2.222811</td>
<td>2.616139</td>
</tr>
<tr>
<td>C</td>
<td>16.962238</td>
<td>-1.013441</td>
<td>2.110651</td>
</tr>
<tr>
<td>C</td>
<td>18.346372</td>
<td>-0.839831</td>
<td>2.041873</td>
</tr>
<tr>
<td>C</td>
<td>18.913528</td>
<td>0.338822</td>
<td>1.554744</td>
</tr>
<tr>
<td>C</td>
<td>20.423743</td>
<td>0.473128</td>
<td>1.597960</td>
</tr>
<tr>
<td>C</td>
<td>20.955100</td>
<td>1.545913</td>
<td>0.658146</td>
</tr>
<tr>
<td>C</td>
<td>20.178753</td>
<td>2.848517</td>
<td>0.819877</td>
</tr>
<tr>
<td>C</td>
<td>18.689704</td>
<td>2.652579</td>
<td>0.516039</td>
</tr>
<tr>
<td>C</td>
<td>18.093707</td>
<td>1.387650</td>
<td>1.106949</td>
</tr>
<tr>
<td>C</td>
<td>16.682292</td>
<td>1.249421</td>
<td>1.166788</td>
</tr>
<tr>
<td>C</td>
<td>15.780028</td>
<td>2.283224</td>
<td>0.729812</td>
</tr>
<tr>
<td>C</td>
<td>14.429430</td>
<td>2.134574</td>
<td>0.807205</td>
</tr>
<tr>
<td>C</td>
<td>13.832894</td>
<td>0.935452</td>
<td>1.318902</td>
</tr>
<tr>
<td>C</td>
<td>14.694485</td>
<td>-0.113995</td>
<td>1.751422</td>
</tr>
<tr>
<td>C</td>
<td>16.111444</td>
<td>0.044257</td>
<td>1.674405</td>
</tr>
<tr>
<td>O</td>
<td>21.022650</td>
<td>-0.793105</td>
<td>1.305426</td>
</tr>
<tr>
<td>O</td>
<td>22.337795</td>
<td>1.723227</td>
<td>1.002001</td>
</tr>
<tr>
<td>O</td>
<td>20.286724</td>
<td>3.347526</td>
<td>2.153463</td>
</tr>
<tr>
<td>H</td>
<td>11.785951</td>
<td>1.561347</td>
<td>1.074737</td>
</tr>
<tr>
<td>H</td>
<td>10.827586</td>
<td>-0.540201</td>
<td>1.964009</td>
</tr>
<tr>
<td>H</td>
<td>12.309728</td>
<td>-2.373524</td>
<td>2.714880</td>
</tr>
<tr>
<td>H</td>
<td>14.590408</td>
<td>-3.289590</td>
<td>3.074088</td>
</tr>
<tr>
<td>H</td>
<td>17.028798</td>
<td>-3.021668</td>
<td>2.943513</td>
</tr>
<tr>
<td>H</td>
<td>18.999140</td>
<td>-1.637377</td>
<td>2.376700</td>
</tr>
<tr>
<td>H</td>
<td>20.706841</td>
<td>0.764019</td>
<td>2.618323</td>
</tr>
<tr>
<td>H</td>
<td>20.872189</td>
<td>1.193458</td>
<td>-0.375918</td>
</tr>
<tr>
<td>H</td>
<td>20.562896</td>
<td>3.593011</td>
<td>0.112585</td>
</tr>
<tr>
<td>H</td>
<td>18.180133</td>
<td>3.531754</td>
<td>0.915767</td>
</tr>
<tr>
<td>H</td>
<td>16.182106</td>
<td>3.198354</td>
<td>0.315556</td>
</tr>
<tr>
<td>H</td>
<td>13.777255</td>
<td>2.935500</td>
<td>0.472031</td>
</tr>
<tr>
<td>H</td>
<td>21.978840</td>
<td>-0.682671</td>
<td>1.396343</td>
</tr>
<tr>
<td>H</td>
<td>22.816744</td>
<td>2.093223</td>
<td>0.250257</td>
</tr>
<tr>
<td>O</td>
<td>18.478256</td>
<td>2.713263</td>
<td>-0.909551</td>
</tr>
<tr>
<td>H</td>
<td>18.484058</td>
<td>1.818907</td>
<td>-1.273862</td>
</tr>
<tr>
<td>H</td>
<td>21.225869</td>
<td>3.372851</td>
<td>2.385325</td>
</tr>
</tbody>
</table>
Table S61: BPW91 6-311g* hydrogen bonded structure (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.583539</td>
<td>4.177554</td>
<td>1.587857</td>
</tr>
<tr>
<td>C</td>
<td>0.069264</td>
<td>2.755728</td>
<td>1.666727</td>
</tr>
<tr>
<td>C</td>
<td>0.518505</td>
<td>1.801080</td>
<td>0.722626</td>
</tr>
<tr>
<td>C</td>
<td>1.597264</td>
<td>2.181878</td>
<td>-0.226470</td>
</tr>
<tr>
<td>C</td>
<td>2.377718</td>
<td>3.415933</td>
<td>-0.001085</td>
</tr>
<tr>
<td>C</td>
<td>2.072804</td>
<td>4.244785</td>
<td>1.222421</td>
</tr>
<tr>
<td>C</td>
<td>-0.023894</td>
<td>0.485381</td>
<td>0.724990</td>
</tr>
<tr>
<td>C</td>
<td>-0.985915</td>
<td>0.129476</td>
<td>1.732924</td>
</tr>
<tr>
<td>C</td>
<td>-1.402832</td>
<td>1.101537</td>
<td>2.698856</td>
</tr>
<tr>
<td>C</td>
<td>-0.871278</td>
<td>2.404135</td>
<td>2.634733</td>
</tr>
<tr>
<td>C</td>
<td>-1.532316</td>
<td>-1.191188</td>
<td>1.780458</td>
</tr>
<tr>
<td>C</td>
<td>-1.133046</td>
<td>-2.170760</td>
<td>0.813779</td>
</tr>
<tr>
<td>C</td>
<td>-0.181333</td>
<td>-1.782586</td>
<td>-0.194990</td>
</tr>
<tr>
<td>C</td>
<td>0.344213</td>
<td>-0.520882</td>
<td>-0.240693</td>
</tr>
<tr>
<td>C</td>
<td>-2.483041</td>
<td>-1.543838</td>
<td>2.796618</td>
</tr>
<tr>
<td>C</td>
<td>-3.002137</td>
<td>-2.855453</td>
<td>2.824017</td>
</tr>
<tr>
<td>C</td>
<td>-2.603981</td>
<td>-3.803447</td>
<td>1.876419</td>
</tr>
<tr>
<td>C</td>
<td>-1.681308</td>
<td>-3.468423</td>
<td>0.880356</td>
</tr>
<tr>
<td>C</td>
<td>-2.357335</td>
<td>0.722536</td>
<td>3.704281</td>
</tr>
<tr>
<td>C</td>
<td>-2.873707</td>
<td>-0.544785</td>
<td>3.752982</td>
</tr>
<tr>
<td>O</td>
<td>1.364919</td>
<td>3.406138</td>
<td>-1.047154</td>
</tr>
<tr>
<td>O</td>
<td>2.357541</td>
<td>5.645808</td>
<td>1.046382</td>
</tr>
<tr>
<td>O</td>
<td>0.356282</td>
<td>4.864661</td>
<td>2.819232</td>
</tr>
<tr>
<td>O</td>
<td>2.640115</td>
<td>3.088889</td>
<td>-3.502388</td>
</tr>
<tr>
<td>As</td>
<td>2.643438</td>
<td>1.355983</td>
<td>-3.982240</td>
</tr>
<tr>
<td>O</td>
<td>2.694459</td>
<td>0.329000</td>
<td>-2.666506</td>
</tr>
<tr>
<td>C</td>
<td>1.056550</td>
<td>1.137497</td>
<td>-5.091372</td>
</tr>
<tr>
<td>C</td>
<td>4.218029</td>
<td>1.331698</td>
<td>-5.118399</td>
</tr>
<tr>
<td>H</td>
<td>-1.193452</td>
<td>3.152909</td>
<td>3.359139</td>
</tr>
<tr>
<td>H</td>
<td>1.044358</td>
<td>-0.276781</td>
<td>-1.042441</td>
</tr>
<tr>
<td>H</td>
<td>0.104494</td>
<td>-2.521176</td>
<td>-0.945861</td>
</tr>
<tr>
<td>H</td>
<td>-1.376277</td>
<td>-4.214065</td>
<td>0.142190</td>
</tr>
<tr>
<td>H</td>
<td>-3.017488</td>
<td>-4.813476</td>
<td>1.914254</td>
</tr>
<tr>
<td>H</td>
<td>-3.724196</td>
<td>-3.125740</td>
<td>3.598285</td>
</tr>
<tr>
<td>H</td>
<td>-3.597560</td>
<td>-0.815385</td>
<td>4.525630</td>
</tr>
<tr>
<td>H</td>
<td>-2.666223</td>
<td>1.472400</td>
<td>4.436635</td>
</tr>
<tr>
<td>H</td>
<td>2.075493</td>
<td>1.398612</td>
<td>-0.818657</td>
</tr>
<tr>
<td>H</td>
<td>3.404263</td>
<td>3.460514</td>
<td>-0.379409</td>
</tr>
<tr>
<td>H</td>
<td>2.659837</td>
<td>3.838983</td>
<td>2.066208</td>
</tr>
<tr>
<td>H</td>
<td>0.040998</td>
<td>4.694407</td>
<td>0.772110</td>
</tr>
<tr>
<td>H</td>
<td>3.291477</td>
<td>5.798875</td>
<td>1.265684</td>
</tr>
<tr>
<td>H</td>
<td>0.790629</td>
<td>5.730391</td>
<td>2.701056</td>
</tr>
<tr>
<td>H</td>
<td>1.069026</td>
<td>1.884331</td>
<td>-5.893554</td>
</tr>
<tr>
<td>H</td>
<td>0.170974</td>
<td>1.275830</td>
<td>-4.460667</td>
</tr>
<tr>
<td>H</td>
<td>1.056992</td>
<td>0.126631</td>
<td>-5.516339</td>
</tr>
<tr>
<td>H</td>
<td>4.135171</td>
<td>2.127335</td>
<td>-5.867723</td>
</tr>
<tr>
<td>H</td>
<td>2.109763</td>
<td>3.210402</td>
<td>-2.668947</td>
</tr>
<tr>
<td>H</td>
<td>4.283008</td>
<td>0.355254</td>
<td>-5.612252</td>
</tr>
<tr>
<td>H</td>
<td>5.100299</td>
<td>1.493649</td>
<td>-4.489380</td>
</tr>
</tbody>
</table>
Table S62: BPW91 6-311+g* hydrogen bonded structure (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.609157</td>
<td>4.178550</td>
<td>1.617049</td>
</tr>
<tr>
<td>C</td>
<td>0.083780</td>
<td>2.758229</td>
<td>1.685293</td>
</tr>
<tr>
<td>C</td>
<td>0.548826</td>
<td>1.798028</td>
<td>0.754311</td>
</tr>
<tr>
<td>C</td>
<td>1.650956</td>
<td>2.167205</td>
<td>-0.170551</td>
</tr>
<tr>
<td>C</td>
<td>2.432381</td>
<td>3.398412</td>
<td>0.063406</td>
</tr>
<tr>
<td>C</td>
<td>2.104270</td>
<td>4.241779</td>
<td>1.270641</td>
</tr>
<tr>
<td>C</td>
<td>0.000071</td>
<td>0.484636</td>
<td>0.747792</td>
</tr>
<tr>
<td>C</td>
<td>-0.988745</td>
<td>0.136631</td>
<td>1.731746</td>
</tr>
<tr>
<td>C</td>
<td>-1.424421</td>
<td>1.114017</td>
<td>2.683503</td>
</tr>
<tr>
<td>C</td>
<td>-0.883932</td>
<td>2.413794</td>
<td>2.629780</td>
</tr>
<tr>
<td>C</td>
<td>-1.541995</td>
<td>-1.181699</td>
<td>1.770779</td>
</tr>
<tr>
<td>C</td>
<td>-1.123434</td>
<td>-2.166601</td>
<td>0.817895</td>
</tr>
<tr>
<td>C</td>
<td>-0.152492</td>
<td>-1.786443</td>
<td>-0.169173</td>
</tr>
<tr>
<td>C</td>
<td>0.386216</td>
<td>-0.526729</td>
<td>-0.205148</td>
</tr>
<tr>
<td>C</td>
<td>-2.518926</td>
<td>-1.526183</td>
<td>2.764533</td>
</tr>
<tr>
<td>C</td>
<td>-3.043849</td>
<td>-2.835911</td>
<td>2.784978</td>
</tr>
<tr>
<td>C</td>
<td>-2.626402</td>
<td>-3.789768</td>
<td>1.850935</td>
</tr>
<tr>
<td>C</td>
<td>-1.678379</td>
<td>-3.462185</td>
<td>0.875778</td>
</tr>
<tr>
<td>C</td>
<td>-2.406393</td>
<td>0.743917</td>
<td>3.665972</td>
</tr>
<tr>
<td>C</td>
<td>-2.929418</td>
<td>-0.521485</td>
<td>3.706882</td>
</tr>
<tr>
<td>O</td>
<td>1.448538</td>
<td>3.833196</td>
<td>-1.010094</td>
</tr>
<tr>
<td>O</td>
<td>2.398492</td>
<td>5.641203</td>
<td>1.079497</td>
</tr>
<tr>
<td>O</td>
<td>0.360218</td>
<td>4.860267</td>
<td>2.851821</td>
</tr>
<tr>
<td>O</td>
<td>2.531261</td>
<td>3.098111</td>
<td>-3.567674</td>
</tr>
<tr>
<td>As</td>
<td>2.656795</td>
<td>1.358472</td>
<td>-4.031122</td>
</tr>
<tr>
<td>O</td>
<td>2.652297</td>
<td>0.964774</td>
<td>-2.698233</td>
</tr>
<tr>
<td>C</td>
<td>1.033981</td>
<td>0.932023</td>
<td>-5.042969</td>
</tr>
<tr>
<td>C</td>
<td>4.170670</td>
<td>1.438475</td>
<td>-5.242959</td>
</tr>
<tr>
<td>H</td>
<td>-1.221894</td>
<td>3.164191</td>
<td>3.345255</td>
</tr>
<tr>
<td>H</td>
<td>1.107880</td>
<td>-0.289311</td>
<td>-0.988806</td>
</tr>
<tr>
<td>H</td>
<td>0.155454</td>
<td>-2.528781</td>
<td>-0.910265</td>
</tr>
<tr>
<td>H</td>
<td>-1.358712</td>
<td>-4.212080</td>
<td>0.147922</td>
</tr>
<tr>
<td>H</td>
<td>-3.044749</td>
<td>-4.798195</td>
<td>1.882803</td>
</tr>
<tr>
<td>H</td>
<td>-3.785880</td>
<td>-3.100269</td>
<td>3.542498</td>
</tr>
<tr>
<td>H</td>
<td>-3.673935</td>
<td>-0.785653</td>
<td>4.462134</td>
</tr>
<tr>
<td>H</td>
<td>-2.730313</td>
<td>1.497958</td>
<td>4.387683</td>
</tr>
<tr>
<td>H</td>
<td>2.414738</td>
<td>1.377198</td>
<td>-0.741421</td>
</tr>
<tr>
<td>H</td>
<td>3.469727</td>
<td>3.431152</td>
<td>-0.285848</td>
</tr>
<tr>
<td>H</td>
<td>2.684525</td>
<td>3.849826</td>
<td>2.125297</td>
</tr>
<tr>
<td>H</td>
<td>0.074894</td>
<td>4.705008</td>
<td>0.802916</td>
</tr>
<tr>
<td>H</td>
<td>3.335552</td>
<td>5.800581</td>
<td>1.294659</td>
</tr>
<tr>
<td>H</td>
<td>0.753241</td>
<td>5.747438</td>
<td>2.747119</td>
</tr>
<tr>
<td>H</td>
<td>0.943409</td>
<td>1.722874</td>
<td>-5.855952</td>
</tr>
<tr>
<td>H</td>
<td>0.177751</td>
<td>1.073348</td>
<td>-4.363621</td>
</tr>
<tr>
<td>H</td>
<td>1.095071</td>
<td>-0.022808</td>
<td>-5.451314</td>
</tr>
<tr>
<td>H</td>
<td>3.982370</td>
<td>2.205641</td>
<td>-6.003239</td>
</tr>
<tr>
<td>H</td>
<td>2.105795</td>
<td>3.190360</td>
<td>-2.671473</td>
</tr>
<tr>
<td>H</td>
<td>4.292395</td>
<td>0.458284</td>
<td>-5.718657</td>
</tr>
<tr>
<td>H</td>
<td>5.065031</td>
<td>1.689578</td>
<td>-4.662033</td>
</tr>
</tbody>
</table>
Table S63: BLYP 6-311g* hydrogen bonded structure (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.583395</td>
<td>4.186837</td>
<td>1.604239</td>
</tr>
<tr>
<td>C</td>
<td>0.071677</td>
<td>2.754893</td>
<td>1.684416</td>
</tr>
<tr>
<td>C</td>
<td>0.523372</td>
<td>1.798123</td>
<td>0.736522</td>
</tr>
<tr>
<td>C</td>
<td>1.607336</td>
<td>2.180110</td>
<td>-0.214554</td>
</tr>
<tr>
<td>C</td>
<td>2.280595</td>
<td>3.426023</td>
<td>-0.003137</td>
</tr>
<tr>
<td>C</td>
<td>2.074192</td>
<td>4.266566</td>
<td>1.219555</td>
</tr>
<tr>
<td>C</td>
<td>-0.022527</td>
<td>0.478595</td>
<td>0.735814</td>
</tr>
<tr>
<td>C</td>
<td>-0.989038</td>
<td>0.121342</td>
<td>1.746301</td>
</tr>
<tr>
<td>C</td>
<td>-1.406184</td>
<td>1.095972</td>
<td>2.716585</td>
</tr>
<tr>
<td>C</td>
<td>-0.871712</td>
<td>2.401193</td>
<td>2.653414</td>
</tr>
<tr>
<td>C</td>
<td>-1.540188</td>
<td>-1.205882</td>
<td>1.791805</td>
</tr>
<tr>
<td>C</td>
<td>-1.141684</td>
<td>-2.184820</td>
<td>0.820454</td>
</tr>
<tr>
<td>C</td>
<td>-0.528400</td>
<td>-1.794524</td>
<td>-0.190170</td>
</tr>
<tr>
<td>C</td>
<td>0.343330</td>
<td>-0.531727</td>
<td>-0.234610</td>
</tr>
<tr>
<td>C</td>
<td>-2.495541</td>
<td>-1.556146</td>
<td>2.810377</td>
</tr>
<tr>
<td>C</td>
<td>-3.018472</td>
<td>-2.870133</td>
<td>2.834642</td>
</tr>
<tr>
<td>C</td>
<td>-2.620915</td>
<td>-3.819555</td>
<td>1.883265</td>
</tr>
<tr>
<td>C</td>
<td>-1.694862</td>
<td>-3.484401</td>
<td>0.885714</td>
</tr>
<tr>
<td>C</td>
<td>-2.365140</td>
<td>0.714928</td>
<td>3.723788</td>
</tr>
<tr>
<td>C</td>
<td>-2.884994</td>
<td>-0.535646</td>
<td>3.770563</td>
</tr>
<tr>
<td>O</td>
<td>1.361821</td>
<td>3.410717</td>
<td>-1.059058</td>
</tr>
<tr>
<td>O</td>
<td>2.343267</td>
<td>5.679426</td>
<td>1.020681</td>
</tr>
<tr>
<td>O</td>
<td>0.366379</td>
<td>4.869149</td>
<td>2.853875</td>
</tr>
<tr>
<td>O</td>
<td>2.666421</td>
<td>3.095796</td>
<td>-3.516107</td>
</tr>
<tr>
<td>As</td>
<td>2.654977</td>
<td>1.351219</td>
<td>-4.053977</td>
</tr>
<tr>
<td>O</td>
<td>2.687585</td>
<td>0.315103</td>
<td>-2.683898</td>
</tr>
<tr>
<td>C</td>
<td>1.655506</td>
<td>1.152772</td>
<td>-5.132969</td>
</tr>
<tr>
<td>C</td>
<td>4.251373</td>
<td>1.318741</td>
<td>-5.141933</td>
</tr>
<tr>
<td>H</td>
<td>-1.194644</td>
<td>3.148792</td>
<td>3.377739</td>
</tr>
<tr>
<td>H</td>
<td>1.042300</td>
<td>-0.289228</td>
<td>-1.036157</td>
</tr>
<tr>
<td>H</td>
<td>-0.083226</td>
<td>-2.323737</td>
<td>-0.092212</td>
</tr>
<tr>
<td>H</td>
<td>-1.391931</td>
<td>-4.230331</td>
<td>0.146944</td>
</tr>
<tr>
<td>H</td>
<td>-3.807333</td>
<td>-4.828550</td>
<td>1.919188</td>
</tr>
<tr>
<td>H</td>
<td>-3.741549</td>
<td>-3.140830</td>
<td>3.607556</td>
</tr>
<tr>
<td>H</td>
<td>-3.609667</td>
<td>-0.823547</td>
<td>4.542431</td>
</tr>
<tr>
<td>H</td>
<td>-2.672975</td>
<td>1.464236</td>
<td>4.456905</td>
</tr>
<tr>
<td>H</td>
<td>2.085971</td>
<td>1.397779</td>
<td>-0.803350</td>
</tr>
<tr>
<td>H</td>
<td>3.406414</td>
<td>3.477459</td>
<td>-0.383104</td>
</tr>
<tr>
<td>H</td>
<td>2.676608</td>
<td>3.882269</td>
<td>2.061442</td>
</tr>
<tr>
<td>H</td>
<td>0.026968</td>
<td>4.709942</td>
<td>0.803891</td>
</tr>
<tr>
<td>H</td>
<td>3.282078</td>
<td>5.844932</td>
<td>1.221882</td>
</tr>
<tr>
<td>H</td>
<td>0.777007</td>
<td>5.748269</td>
<td>2.732570</td>
</tr>
<tr>
<td>H</td>
<td>1.079535</td>
<td>1.905839</td>
<td>-5.928892</td>
</tr>
<tr>
<td>H</td>
<td>0.170309</td>
<td>1.295644</td>
<td>-4.502921</td>
</tr>
<tr>
<td>H</td>
<td>1.049454</td>
<td>0.144671</td>
<td>-5.564012</td>
</tr>
<tr>
<td>H</td>
<td>4.183668</td>
<td>2.127637</td>
<td>-5.878316</td>
</tr>
<tr>
<td>H</td>
<td>2.124648</td>
<td>3.223178</td>
<td>-2.689228</td>
</tr>
<tr>
<td>H</td>
<td>4.302576</td>
<td>0.348731</td>
<td>-5.649604</td>
</tr>
<tr>
<td>H</td>
<td>5.131106</td>
<td>1.457275</td>
<td>-4.504028</td>
</tr>
</tbody>
</table>
Table S64: BLYP 6-311+g* hydrogen bonded structure (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.614668</td>
<td>4.191351</td>
<td>1.664640</td>
</tr>
<tr>
<td>C</td>
<td>0.091828</td>
<td>2.760099</td>
<td>1.711785</td>
</tr>
<tr>
<td>C</td>
<td>0.565410</td>
<td>1.797511</td>
<td>0.780114</td>
</tr>
<tr>
<td>C</td>
<td>1.676489</td>
<td>2.168093</td>
<td>-0.141408</td>
</tr>
<tr>
<td>C</td>
<td>2.448290</td>
<td>3.412169</td>
<td>0.079595</td>
</tr>
<tr>
<td>C</td>
<td>2.111930</td>
<td>4.270099</td>
<td>1.281860</td>
</tr>
<tr>
<td>C</td>
<td>0.013185</td>
<td>0.480127</td>
<td>0.766905</td>
</tr>
<tr>
<td>C</td>
<td>-0.988631</td>
<td>0.131310</td>
<td>1.744775</td>
</tr>
<tr>
<td>C</td>
<td>-1.432228</td>
<td>1.111695</td>
<td>2.696891</td>
</tr>
<tr>
<td>C</td>
<td>-0.887109</td>
<td>2.413760</td>
<td>2.649145</td>
</tr>
<tr>
<td>C</td>
<td>-1.548111</td>
<td>-1.189921</td>
<td>1.776524</td>
</tr>
<tr>
<td>C</td>
<td>-1.122244</td>
<td>-2.177891</td>
<td>0.822812</td>
</tr>
<tr>
<td>C</td>
<td>-0.137169</td>
<td>-1.796898</td>
<td>-0.156544</td>
</tr>
<tr>
<td>C</td>
<td>0.406293</td>
<td>-0.536136</td>
<td>-0.186183</td>
</tr>
<tr>
<td>C</td>
<td>-2.539242</td>
<td>-1.534364</td>
<td>2.763478</td>
</tr>
<tr>
<td>C</td>
<td>-3.069863</td>
<td>-2.845934</td>
<td>2.775564</td>
</tr>
<tr>
<td>C</td>
<td>-2.645225</td>
<td>-3.801727</td>
<td>1.841304</td>
</tr>
<tr>
<td>C</td>
<td>-1.684085</td>
<td>-3.474943</td>
<td>0.873646</td>
</tr>
<tr>
<td>C</td>
<td>-2.427887</td>
<td>0.740465</td>
<td>3.672365</td>
</tr>
<tr>
<td>C</td>
<td>-2.956262</td>
<td>-0.525750</td>
<td>3.706137</td>
</tr>
<tr>
<td>O</td>
<td>1.464647</td>
<td>3.888070</td>
<td>-1.009997</td>
</tr>
<tr>
<td>O</td>
<td>2.388994</td>
<td>5.881609</td>
<td>1.061445</td>
</tr>
<tr>
<td>O</td>
<td>0.373624</td>
<td>4.863602</td>
<td>2.903483</td>
</tr>
<tr>
<td>O</td>
<td>2.544544</td>
<td>3.096490</td>
<td>-3.590613</td>
</tr>
<tr>
<td>As</td>
<td>2.665442</td>
<td>1.342038</td>
<td>-4.062566</td>
</tr>
<tr>
<td>O</td>
<td>2.874159</td>
<td>0.340645</td>
<td>-2.724946</td>
</tr>
<tr>
<td>C</td>
<td>1.016683</td>
<td>0.978773</td>
<td>-5.068673</td>
</tr>
<tr>
<td>C</td>
<td>4.185101</td>
<td>1.430752</td>
<td>-5.298099</td>
</tr>
<tr>
<td>H</td>
<td>-1.231484</td>
<td>3.162537</td>
<td>3.362033</td>
</tr>
<tr>
<td>H</td>
<td>1.135657</td>
<td>-0.301388</td>
<td>-0.961709</td>
</tr>
<tr>
<td>H</td>
<td>0.176391</td>
<td>-2.538855</td>
<td>-0.895169</td>
</tr>
<tr>
<td>H</td>
<td>-1.360629</td>
<td>-4.224910</td>
<td>0.148111</td>
</tr>
<tr>
<td>H</td>
<td>-3.067305</td>
<td>-4.808420</td>
<td>1.866992</td>
</tr>
<tr>
<td>H</td>
<td>-3.820196</td>
<td>-3.109852</td>
<td>3.524481</td>
</tr>
<tr>
<td>H</td>
<td>-3.708665</td>
<td>-0.788469</td>
<td>4.453536</td>
</tr>
<tr>
<td>H</td>
<td>-2.756470</td>
<td>1.493917</td>
<td>4.392037</td>
</tr>
<tr>
<td>H</td>
<td>2.171236</td>
<td>1.378518</td>
<td>-0.705191</td>
</tr>
<tr>
<td>H</td>
<td>3.486491</td>
<td>3.452144</td>
<td>-0.265231</td>
</tr>
<tr>
<td>H</td>
<td>2.707982</td>
<td>3.905541</td>
<td>2.136293</td>
</tr>
<tr>
<td>H</td>
<td>0.064768</td>
<td>4.726672</td>
<td>0.851154</td>
</tr>
<tr>
<td>H</td>
<td>3.328517</td>
<td>5.856872</td>
<td>1.257259</td>
</tr>
<tr>
<td>H</td>
<td>0.723467</td>
<td>5.770827</td>
<td>2.797759</td>
</tr>
<tr>
<td>H</td>
<td>0.922188</td>
<td>1.711686</td>
<td>-5.877996</td>
</tr>
<tr>
<td>H</td>
<td>0.169319</td>
<td>1.059884</td>
<td>-4.378736</td>
</tr>
<tr>
<td>H</td>
<td>1.073952</td>
<td>-0.036487</td>
<td>-5.478824</td>
</tr>
<tr>
<td>H</td>
<td>3.988756</td>
<td>2.204653</td>
<td>-6.049240</td>
</tr>
<tr>
<td>H</td>
<td>2.125557</td>
<td>3.192237</td>
<td>-2.690314</td>
</tr>
<tr>
<td>H</td>
<td>4.299947</td>
<td>0.453636</td>
<td>-5.781379</td>
</tr>
<tr>
<td>H</td>
<td>5.083061</td>
<td>1.676400</td>
<td>-4.720779</td>
</tr>
</tbody>
</table>
Table S65: B1LYP 6-311g* hydrogen bonded structure (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.594154</td>
<td>4.168896</td>
<td>1.596281</td>
</tr>
<tr>
<td>C</td>
<td>0.079919</td>
<td>2.747202</td>
<td>1.669151</td>
</tr>
<tr>
<td>C</td>
<td>0.537611</td>
<td>1.795518</td>
<td>0.737957</td>
</tr>
<tr>
<td>C</td>
<td>1.625515</td>
<td>2.177869</td>
<td>-0.201683</td>
</tr>
<tr>
<td>C</td>
<td>2.396572</td>
<td>3.405964</td>
<td>0.027819</td>
</tr>
<tr>
<td>C</td>
<td>2.079506</td>
<td>4.240525</td>
<td>1.239572</td>
</tr>
<tr>
<td>C</td>
<td>-0.000268</td>
<td>0.488064</td>
<td>0.735292</td>
</tr>
<tr>
<td>C</td>
<td>-0.971821</td>
<td>0.136157</td>
<td>1.723827</td>
</tr>
<tr>
<td>C</td>
<td>-1.400708</td>
<td>1.104472</td>
<td>2.675391</td>
</tr>
<tr>
<td>C</td>
<td>-0.870842</td>
<td>2.399435</td>
<td>2.618876</td>
</tr>
<tr>
<td>C</td>
<td>-1.518122</td>
<td>-1.182297</td>
<td>1.766355</td>
</tr>
<tr>
<td>C</td>
<td>-1.106553</td>
<td>-2.150505</td>
<td>0.813602</td>
</tr>
<tr>
<td>C</td>
<td>-0.147872</td>
<td>-1.771612</td>
<td>-0.182074</td>
</tr>
<tr>
<td>C</td>
<td>0.380714</td>
<td>-0.520684</td>
<td>-0.224028</td>
</tr>
<tr>
<td>C</td>
<td>-2.478338</td>
<td>-1.530224</td>
<td>2.763069</td>
</tr>
<tr>
<td>C</td>
<td>-2.995405</td>
<td>-2.833944</td>
<td>2.786680</td>
</tr>
<tr>
<td>C</td>
<td>-2.584793</td>
<td>-3.779926</td>
<td>1.852182</td>
</tr>
<tr>
<td>C</td>
<td>-1.651733</td>
<td>-3.448418</td>
<td>0.873948</td>
</tr>
<tr>
<td>C</td>
<td>-2.370724</td>
<td>0.727794</td>
<td>3.666360</td>
</tr>
<tr>
<td>C</td>
<td>-2.883505</td>
<td>-0.528640</td>
<td>3.710039</td>
</tr>
<tr>
<td>O</td>
<td>1.399389</td>
<td>3.386025</td>
<td>-1.016411</td>
</tr>
<tr>
<td>O</td>
<td>2.359211</td>
<td>5.629810</td>
<td>1.048076</td>
</tr>
<tr>
<td>O</td>
<td>0.361889</td>
<td>4.839966</td>
<td>2.826984</td>
</tr>
<tr>
<td>O</td>
<td>2.594760</td>
<td>3.063883</td>
<td>-3.509375</td>
</tr>
<tr>
<td>As</td>
<td>2.605966</td>
<td>1.350890</td>
<td>-3.980443</td>
</tr>
<tr>
<td>O</td>
<td>2.657027</td>
<td>0.349265</td>
<td>-2.662864</td>
</tr>
<tr>
<td>C</td>
<td>1.921854</td>
<td>1.129707</td>
<td>-5.071756</td>
</tr>
<tr>
<td>C</td>
<td>4.173700</td>
<td>1.314702</td>
<td>-5.107876</td>
</tr>
<tr>
<td>H</td>
<td>-1.206661</td>
<td>3.142940</td>
<td>3.32246</td>
</tr>
<tr>
<td>H</td>
<td>1.084128</td>
<td>-0.279639</td>
<td>-1.011149</td>
</tr>
<tr>
<td>H</td>
<td>0.151683</td>
<td>-2.507334</td>
<td>-0.921006</td>
</tr>
<tr>
<td>H</td>
<td>-1.338440</td>
<td>-4.190505</td>
<td>0.147882</td>
</tr>
<tr>
<td>H</td>
<td>-2.995617</td>
<td>-4.782348</td>
<td>1.885946</td>
</tr>
<tr>
<td>H</td>
<td>-3.723845</td>
<td>-3.100707</td>
<td>3.544463</td>
</tr>
<tr>
<td>H</td>
<td>-3.613887</td>
<td>-0.796343</td>
<td>4.465739</td>
</tr>
<tr>
<td>H</td>
<td>-2.687440</td>
<td>1.474782</td>
<td>4.385918</td>
</tr>
<tr>
<td>H</td>
<td>2.103576</td>
<td>1.398918</td>
<td>-0.779604</td>
</tr>
<tr>
<td>H</td>
<td>3.417434</td>
<td>3.458006</td>
<td>-0.340130</td>
</tr>
<tr>
<td>H</td>
<td>2.660238</td>
<td>3.851931</td>
<td>2.084029</td>
</tr>
<tr>
<td>H</td>
<td>0.055956</td>
<td>4.688649</td>
<td>0.793613</td>
</tr>
<tr>
<td>H</td>
<td>3.290469</td>
<td>5.794543</td>
<td>1.224058</td>
</tr>
<tr>
<td>H</td>
<td>0.747085</td>
<td>5.718643</td>
<td>2.727081</td>
</tr>
<tr>
<td>H</td>
<td>1.025055</td>
<td>1.865891</td>
<td>-5.871251</td>
</tr>
<tr>
<td>H</td>
<td>0.145340</td>
<td>1.264815</td>
<td>-4.440855</td>
</tr>
<tr>
<td>H</td>
<td>1.017690</td>
<td>0.122624</td>
<td>-5.492560</td>
</tr>
<tr>
<td>H</td>
<td>4.094506</td>
<td>2.096284</td>
<td>-5.861541</td>
</tr>
<tr>
<td>H</td>
<td>2.103749</td>
<td>3.207734</td>
<td>-2.673158</td>
</tr>
<tr>
<td>H</td>
<td>4.242584</td>
<td>0.340587</td>
<td>-5.589228</td>
</tr>
<tr>
<td>H</td>
<td>5.050178</td>
<td>1.483046</td>
<td>-4.485123</td>
</tr>
</tbody>
</table>
Table S66: BPW91 6-311g* hydrogen bonded structure (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.621056</td>
<td>4.177330</td>
<td>1.629155</td>
</tr>
<tr>
<td>C</td>
<td>0.099911</td>
<td>2.755460</td>
<td>1.688219</td>
</tr>
<tr>
<td>C</td>
<td>0.583567</td>
<td>1.798508</td>
<td>0.773586</td>
</tr>
<tr>
<td>C</td>
<td>1.698563</td>
<td>2.172670</td>
<td>-0.133879</td>
</tr>
<tr>
<td>C</td>
<td>2.464080</td>
<td>3.401188</td>
<td>0.106872</td>
</tr>
<tr>
<td>C</td>
<td>2.114189</td>
<td>4.249651</td>
<td>1.299713</td>
</tr>
<tr>
<td>C</td>
<td>0.043527</td>
<td>0.491550</td>
<td>0.761378</td>
</tr>
<tr>
<td>C</td>
<td>-0.963479</td>
<td>0.146515</td>
<td>1.715838</td>
</tr>
<tr>
<td>C</td>
<td>-1.422754</td>
<td>1.120435</td>
<td>2.646976</td>
</tr>
<tr>
<td>C</td>
<td>-0.885651</td>
<td>2.413544</td>
<td>2.605341</td>
</tr>
<tr>
<td>C</td>
<td>-1.514335</td>
<td>-1.170764</td>
<td>1.745380</td>
</tr>
<tr>
<td>C</td>
<td>-1.070826</td>
<td>-2.152490</td>
<td>0.813285</td>
</tr>
<tr>
<td>C</td>
<td>-0.075569</td>
<td>-1.773740</td>
<td>-0.149159</td>
</tr>
<tr>
<td>C</td>
<td>0.456495</td>
<td>-0.523240</td>
<td>-0.177927</td>
</tr>
<tr>
<td>C</td>
<td>-2.511178</td>
<td>-1.511035</td>
<td>2.708188</td>
</tr>
<tr>
<td>C</td>
<td>-3.032344</td>
<td>-2.813774</td>
<td>2.729239</td>
</tr>
<tr>
<td>C</td>
<td>-2.590038</td>
<td>-3.766297</td>
<td>1.806018</td>
</tr>
<tr>
<td>C</td>
<td>-1.620851</td>
<td>-3.441867</td>
<td>0.860154</td>
</tr>
<tr>
<td>C</td>
<td>-2.430101</td>
<td>0.752014</td>
<td>3.603821</td>
</tr>
<tr>
<td>C</td>
<td>-2.948318</td>
<td>-0.503406</td>
<td>3.634744</td>
</tr>
<tr>
<td>O</td>
<td>1.501295</td>
<td>3.371111</td>
<td>-0.969316</td>
</tr>
<tr>
<td>O</td>
<td>2.399980</td>
<td>5.637723</td>
<td>1.093564</td>
</tr>
<tr>
<td>O</td>
<td>0.359242</td>
<td>4.842589</td>
<td>2.860943</td>
</tr>
<tr>
<td>O</td>
<td>2.494174</td>
<td>3.054921</td>
<td>-3.560579</td>
</tr>
<tr>
<td>As</td>
<td>2.587441</td>
<td>1.334537</td>
<td>-4.018990</td>
</tr>
<tr>
<td>O</td>
<td>2.766617</td>
<td>0.359550</td>
<td>-2.686648</td>
</tr>
<tr>
<td>C</td>
<td>0.958381</td>
<td>0.999347</td>
<td>-5.009027</td>
</tr>
<tr>
<td>C</td>
<td>4.094376</td>
<td>1.372240</td>
<td>-5.224951</td>
</tr>
<tr>
<td>H</td>
<td>-1.239163</td>
<td>3.158697</td>
<td>3.305425</td>
</tr>
<tr>
<td>H</td>
<td>1.189275</td>
<td>-0.288459</td>
<td>-0.939160</td>
</tr>
<tr>
<td>H</td>
<td>0.249549</td>
<td>-2.513810</td>
<td>-0.872716</td>
</tr>
<tr>
<td>H</td>
<td>-1.283383</td>
<td>-4.188500</td>
<td>0.149701</td>
</tr>
<tr>
<td>H</td>
<td>-3.004312</td>
<td>-4.767604</td>
<td>1.830087</td>
</tr>
<tr>
<td>H</td>
<td>-3.788762</td>
<td>-3.074775</td>
<td>3.452245</td>
</tr>
<tr>
<td>H</td>
<td>-3.707057</td>
<td>-0.764962</td>
<td>4.364233</td>
</tr>
<tr>
<td>H</td>
<td>-2.770643</td>
<td>1.503122</td>
<td>4.308069</td>
</tr>
<tr>
<td>H</td>
<td>2.193639</td>
<td>1.387920</td>
<td>-0.688206</td>
</tr>
<tr>
<td>H</td>
<td>3.496799</td>
<td>3.446156</td>
<td>-0.227194</td>
</tr>
<tr>
<td>H</td>
<td>2.684008</td>
<td>3.876981</td>
<td>2.158230</td>
</tr>
<tr>
<td>H</td>
<td>0.094123</td>
<td>4.703876</td>
<td>0.824313</td>
</tr>
<tr>
<td>H</td>
<td>3.330186</td>
<td>5.812222</td>
<td>1.271924</td>
</tr>
<tr>
<td>H</td>
<td>0.691286</td>
<td>5.744375</td>
<td>2.772500</td>
</tr>
<tr>
<td>H</td>
<td>0.871516</td>
<td>1.723887</td>
<td>-5.816905</td>
</tr>
<tr>
<td>H</td>
<td>0.115046</td>
<td>1.094856</td>
<td>-4.327279</td>
</tr>
<tr>
<td>H</td>
<td>0.993805</td>
<td>-0.010587</td>
<td>-5.415145</td>
</tr>
<tr>
<td>H</td>
<td>3.925469</td>
<td>2.131374</td>
<td>-5.987080</td>
</tr>
<tr>
<td>H</td>
<td>2.111819</td>
<td>3.181439</td>
<td>-2.665673</td>
</tr>
<tr>
<td>H</td>
<td>4.197880</td>
<td>0.393595</td>
<td>-5.690912</td>
</tr>
<tr>
<td>H</td>
<td>4.988347</td>
<td>1.608163</td>
<td>-4.650876</td>
</tr>
</tbody>
</table>
Table S67: B3LYP 6-311g* hydrogen bonded structure (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.868622</td>
<td>2.405852</td>
<td>2.621295</td>
</tr>
<tr>
<td>C</td>
<td>0.087685</td>
<td>2.754647</td>
<td>1.67976</td>
</tr>
<tr>
<td>C</td>
<td>0.549522</td>
<td>1.804213</td>
<td>0.745485</td>
</tr>
<tr>
<td>C</td>
<td>0.008303</td>
<td>0.497148</td>
<td>0.735614</td>
</tr>
<tr>
<td>C</td>
<td>0.391508</td>
<td>-0.508513</td>
<td>-0.224734</td>
</tr>
<tr>
<td>C</td>
<td>-0.140230</td>
<td>-1.759792</td>
<td>-0.189299</td>
</tr>
<tr>
<td>C</td>
<td>-1.103409</td>
<td>-2.147417</td>
<td>0.800513</td>
</tr>
<tr>
<td>C</td>
<td>-1.651482</td>
<td>-3.437620</td>
<td>0.854815</td>
</tr>
<tr>
<td>C</td>
<td>-2.589444</td>
<td>-3.770671</td>
<td>1.828448</td>
</tr>
<tr>
<td>C</td>
<td>-3.002659</td>
<td>-2.826643</td>
<td>2.764421</td>
</tr>
<tr>
<td>C</td>
<td>-2.483418</td>
<td>-1.522915</td>
<td>2.747162</td>
</tr>
<tr>
<td>C</td>
<td>-2.890922</td>
<td>-0.524044</td>
<td>3.694849</td>
</tr>
<tr>
<td>C</td>
<td>-2.375547</td>
<td>0.733007</td>
<td>3.657116</td>
</tr>
<tr>
<td>C</td>
<td>-1.401116</td>
<td>1.110930</td>
<td>2.672093</td>
</tr>
<tr>
<td>C</td>
<td>-0.969171</td>
<td>0.143988</td>
<td>1.719035</td>
</tr>
<tr>
<td>C</td>
<td>-1.517729</td>
<td>-1.173253</td>
<td>1.755056</td>
</tr>
<tr>
<td>C</td>
<td>1.644990</td>
<td>2.185140</td>
<td>-0.184183</td>
</tr>
<tr>
<td>C</td>
<td>2.418170</td>
<td>3.411490</td>
<td>0.053466</td>
</tr>
<tr>
<td>C</td>
<td>2.093607</td>
<td>4.243593</td>
<td>1.264883</td>
</tr>
<tr>
<td>C</td>
<td>0.604993</td>
<td>4.174904</td>
<td>1.610008</td>
</tr>
<tr>
<td>O</td>
<td>1.429190</td>
<td>3.397827</td>
<td>-1.001235</td>
</tr>
<tr>
<td>O</td>
<td>2.378193</td>
<td>5.634047</td>
<td>1.081267</td>
</tr>
<tr>
<td>O</td>
<td>0.364322</td>
<td>4.847190</td>
<td>2.839152</td>
</tr>
<tr>
<td>H</td>
<td>-1.200883</td>
<td>3.149050</td>
<td>3.335704</td>
</tr>
<tr>
<td>H</td>
<td>1.099565</td>
<td>-0.265833</td>
<td>-1.009088</td>
</tr>
<tr>
<td>H</td>
<td>0.161437</td>
<td>-2.494321</td>
<td>-0.930241</td>
</tr>
<tr>
<td>H</td>
<td>-1.335973</td>
<td>-4.178685</td>
<td>0.126974</td>
</tr>
<tr>
<td>H</td>
<td>-3.002407</td>
<td>-7.735753</td>
<td>1.857447</td>
</tr>
<tr>
<td>H</td>
<td>-3.735482</td>
<td>-3.094733</td>
<td>3.519130</td>
</tr>
<tr>
<td>H</td>
<td>-3.625814</td>
<td>-0.793014</td>
<td>4.447358</td>
</tr>
<tr>
<td>H</td>
<td>-2.694733</td>
<td>1.479027</td>
<td>4.378307</td>
</tr>
<tr>
<td>H</td>
<td>2.125871</td>
<td>1.405665</td>
<td>-0.761839</td>
</tr>
<tr>
<td>H</td>
<td>3.443953</td>
<td>3.460386</td>
<td>-0.304686</td>
</tr>
<tr>
<td>H</td>
<td>2.666871</td>
<td>3.849531</td>
<td>2.113575</td>
</tr>
<tr>
<td>H</td>
<td>0.074397</td>
<td>4.696398</td>
<td>0.801393</td>
</tr>
<tr>
<td>H</td>
<td>3.309345</td>
<td>5.795414</td>
<td>1.269638</td>
</tr>
<tr>
<td>H</td>
<td>0.761618</td>
<td>5.722906</td>
<td>2.742143</td>
</tr>
<tr>
<td>H</td>
<td>0.977302</td>
<td>1.761426</td>
<td>-5.880936</td>
</tr>
<tr>
<td>H</td>
<td>0.129219</td>
<td>1.130130</td>
<td>-4.442377</td>
</tr>
<tr>
<td>H</td>
<td>1.058980</td>
<td>0.022287</td>
<td>-5.485554</td>
</tr>
<tr>
<td>C</td>
<td>1.011570</td>
<td>1.030410</td>
<td>-5.073731</td>
</tr>
<tr>
<td>As</td>
<td>2.583443</td>
<td>1.347803</td>
<td>-3.986251</td>
</tr>
<tr>
<td>H</td>
<td>4.040436</td>
<td>2.118553</td>
<td>-5.885093</td>
</tr>
<tr>
<td>O</td>
<td>2.479926</td>
<td>3.069007</td>
<td>-3.549451</td>
</tr>
<tr>
<td>H</td>
<td>2.107521</td>
<td>3.185180</td>
<td>-2.646772</td>
</tr>
<tr>
<td>H</td>
<td>4.248974</td>
<td>0.371243</td>
<td>-5.588767</td>
</tr>
<tr>
<td>C</td>
<td>4.149147</td>
<td>1.350060</td>
<td>-5.120221</td>
</tr>
<tr>
<td>O</td>
<td>2.683414</td>
<td>0.377767</td>
<td>-2.645510</td>
</tr>
<tr>
<td>H</td>
<td>5.022448</td>
<td>1.557043</td>
<td>-4.503033</td>
</tr>
</tbody>
</table>
Table S68: B3LYP 6-311+g* hydrogen bonded structure (Å).

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.618214</td>
<td>4.178799</td>
<td>1.627824</td>
</tr>
<tr>
<td>C</td>
<td>0.098051</td>
<td>2.757215</td>
<td>1.687480</td>
</tr>
<tr>
<td>C</td>
<td>0.577703</td>
<td>1.801961</td>
<td>0.769714</td>
</tr>
<tr>
<td>C</td>
<td>1.689677</td>
<td>2.176296</td>
<td>-0.141480</td>
</tr>
<tr>
<td>C</td>
<td>2.456625</td>
<td>3.405436</td>
<td>0.098010</td>
</tr>
<tr>
<td>C</td>
<td>2.110416</td>
<td>4.252082</td>
<td>1.293105</td>
</tr>
<tr>
<td>C</td>
<td>0.036434</td>
<td>0.494500</td>
<td>0.754558</td>
</tr>
<tr>
<td>C</td>
<td>-0.965221</td>
<td>0.146746</td>
<td>1.714867</td>
</tr>
<tr>
<td>C</td>
<td>-1.418836</td>
<td>1.118752</td>
<td>2.652239</td>
</tr>
<tr>
<td>C</td>
<td>-0.882274</td>
<td>2.412822</td>
<td>2.609854</td>
</tr>
<tr>
<td>C</td>
<td>-1.515636</td>
<td>-1.170218</td>
<td>1.744174</td>
</tr>
<tr>
<td>C</td>
<td>-1.078303</td>
<td>-2.149720</td>
<td>0.805465</td>
</tr>
<tr>
<td>C</td>
<td>-0.090223</td>
<td>-1.768182</td>
<td>-0.162160</td>
</tr>
<tr>
<td>C</td>
<td>0.442621</td>
<td>-0.516525</td>
<td>-0.190357</td>
</tr>
<tr>
<td>C</td>
<td>-2.506402</td>
<td>-1.513747</td>
<td>2.713424</td>
</tr>
<tr>
<td>C</td>
<td>-3.027261</td>
<td>-2.817361</td>
<td>2.725046</td>
</tr>
<tr>
<td>C</td>
<td>-2.591096</td>
<td>-3.767295</td>
<td>1.804584</td>
</tr>
<tr>
<td>C</td>
<td>-1.628379</td>
<td>-3.439845</td>
<td>0.852581</td>
</tr>
<tr>
<td>C</td>
<td>-2.419024</td>
<td>0.747544</td>
<td>3.614310</td>
</tr>
<tr>
<td>C</td>
<td>-2.937071</td>
<td>-0.509394</td>
<td>3.645362</td>
</tr>
<tr>
<td>O</td>
<td>1.490926</td>
<td>3.377643</td>
<td>-0.977743</td>
</tr>
<tr>
<td>O</td>
<td>2.394835</td>
<td>5.642040</td>
<td>1.089586</td>
</tr>
<tr>
<td>O</td>
<td>0.359794</td>
<td>4.845146</td>
<td>2.860709</td>
</tr>
<tr>
<td>O</td>
<td>2.499313</td>
<td>3.056406</td>
<td>-3.556004</td>
</tr>
<tr>
<td>As</td>
<td>2.592631</td>
<td>1.331901</td>
<td>-4.010221</td>
</tr>
<tr>
<td>O</td>
<td>2.767065</td>
<td>0.357074</td>
<td>-2.674767</td>
</tr>
<tr>
<td>C</td>
<td>0.966193</td>
<td>0.994988</td>
<td>-5.006368</td>
</tr>
<tr>
<td>C</td>
<td>4.103905</td>
<td>1.367464</td>
<td>-5.212576</td>
</tr>
<tr>
<td>H</td>
<td>-1.232235</td>
<td>3.157330</td>
<td>3.314286</td>
</tr>
<tr>
<td>H</td>
<td>1.171218</td>
<td>-0.279151</td>
<td>-0.956800</td>
</tr>
<tr>
<td>H</td>
<td>0.230103</td>
<td>-2.506588</td>
<td>-0.891287</td>
</tr>
<tr>
<td>H</td>
<td>-1.295397</td>
<td>-4.185027</td>
<td>0.136752</td>
</tr>
<tr>
<td>H</td>
<td>-3.005432</td>
<td>-4.769803</td>
<td>1.828631</td>
</tr>
<tr>
<td>H</td>
<td>-3.779219</td>
<td>-3.080911</td>
<td>3.462416</td>
</tr>
<tr>
<td>H</td>
<td>-3.691433</td>
<td>-0.773343</td>
<td>4.380228</td>
</tr>
<tr>
<td>H</td>
<td>-2.755546</td>
<td>1.497256</td>
<td>4.323740</td>
</tr>
<tr>
<td>H</td>
<td>2.184426</td>
<td>1.391214</td>
<td>-0.698626</td>
</tr>
<tr>
<td>H</td>
<td>3.489953</td>
<td>3.449129</td>
<td>-0.238360</td>
</tr>
<tr>
<td>H</td>
<td>2.683676</td>
<td>3.877085</td>
<td>2.149952</td>
</tr>
<tr>
<td>H</td>
<td>0.088348</td>
<td>4.705609</td>
<td>0.823083</td>
</tr>
<tr>
<td>H</td>
<td>3.326526</td>
<td>5.816221</td>
<td>1.269644</td>
</tr>
<tr>
<td>H</td>
<td>0.700624</td>
<td>5.745534</td>
<td>2.770875</td>
</tr>
<tr>
<td>H</td>
<td>0.883221</td>
<td>1.785156</td>
<td>-5.816819</td>
</tr>
<tr>
<td>H</td>
<td>0.119702</td>
<td>1.092630</td>
<td>-4.327357</td>
</tr>
<tr>
<td>H</td>
<td>1.003232</td>
<td>-0.016837</td>
<td>-5.410189</td>
</tr>
<tr>
<td>H</td>
<td>3.937072</td>
<td>2.126912</td>
<td>-5.976206</td>
</tr>
<tr>
<td>H</td>
<td>2.108628</td>
<td>3.183197</td>
<td>-2.661602</td>
</tr>
<tr>
<td>H</td>
<td>4.207652</td>
<td>0.387419</td>
<td>-5.677332</td>
</tr>
<tr>
<td>H</td>
<td>4.997078</td>
<td>1.603383</td>
<td>-4.635523</td>
</tr>
</tbody>
</table>
References

