Photophysics and Photochemistry of cis-trans-Hydroquinone, Catechol and Their Ammonia Clusters: A Theoretical Study

Mitra Ataelahi, Reza Omidyan and Gholamhasan Azimi

Department of Chemistry, University of Isfahan, 81746-73441 Isfahan, Iran.

This supplementary material section contains one Figure and two Tables:

**Figure SM1**: Optimized structures of HQ and CTC monomers and their cluster systems with 1-4 ammonia molecules at the CC2/aug-cc-pVDZ level of theory. Only the $S_2 ({}^1A'')$ excited state, which is accompanied with hydrogen detachment (or transfer) has been depicted. The circles or ellipses have been used to specify HD/HT phenomena.

**Table SM1**: Vertical transition energies of HQ/CTC monomers, and their ammoniated clusters, computed at the CC2/TZVP level of theory.

**Table SM2**: xyz coordinates of the optimized ground state geometry of HQ/CTC monomers, and their ammoniated clusters.
**Figure SM1:**

<table>
<thead>
<tr>
<th></th>
<th>$n=0$</th>
<th>$n=2$</th>
<th>$n=4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>tHQ-(NH$_3$)$_n$</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
</tr>
<tr>
<td>cHQ-(NH$_3$)$_n$</td>
<td><img src="image4.png" alt="Image" /></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
</tr>
<tr>
<td>CTC-(NH$_3$)$_n$</td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
<td><img src="image9.png" alt="Image" /></td>
</tr>
</tbody>
</table>
Table SM1:

<table>
<thead>
<tr>
<th>State</th>
<th>Energy/eV</th>
<th>Oscillator Strength</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>tHQ</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A'1 (\pi_1/\pi_1^<em>), (\pi_2/\pi_2^</em>)</td>
<td>4.63</td>
<td>0.0629</td>
<td>5a*-6a&quot;(84.1%), 4a*-7a&quot;(12.2%)</td>
</tr>
<tr>
<td>A'2 (\pi_1/\pi_1^<em>), (\pi_2/\pi_2^</em>)</td>
<td>6.25</td>
<td>0.1697</td>
<td>5a*-7a&quot;(79.2%), 4a*-6a&quot;(15.1%)</td>
</tr>
<tr>
<td>A'3 (\pi_1/\pi_1^<em>), (\pi_2/\pi_2^</em>)</td>
<td>7.20</td>
<td>0.6970</td>
<td>4a*-6a&quot;(80.5%), 5a*-7a&quot;(12.4%)</td>
</tr>
<tr>
<td>A'4 (\pi_1/\pi_1^<em>), (\pi_2/\pi_2^</em>)</td>
<td>7.48</td>
<td>0.4225</td>
<td>4a*-7a&quot;(80.9%), 5a*-6a&quot;(10.3%)</td>
</tr>
<tr>
<td>A'5 (\pi_1/\pi_1^<em>), (\pi_2/\pi_2^</em>)</td>
<td>7.72</td>
<td>0.0000</td>
<td>3a*-6a&quot;(94.5%), 1a*-6a&quot;(2.0%)</td>
</tr>
<tr>
<td>A''1 (\sigma_1/\sigma_1^<em>), (\pi_2/\sigma_2^</em>)</td>
<td>6.06</td>
<td>0.00009</td>
<td>5a&quot;-25a'(86.2%), 2a&quot;-25a'(4.1%)</td>
</tr>
<tr>
<td>A''2 (\pi_1/\sigma_1^<em>), (\pi_2/\sigma_2^</em>)</td>
<td>6.32</td>
<td>0.0000</td>
<td>5a&quot;-26a'(84.2%), 3a&quot;-25a'(5.5%)</td>
</tr>
<tr>
<td>A''3 (\pi/\sigma_1^<em>), (\pi/\sigma_2^</em>)</td>
<td>7.04</td>
<td>0.0000</td>
<td>5a&quot;-27a'(87.0%), 5a&quot;-36a&quot;(2.7%)</td>
</tr>
<tr>
<td>A''4 (\pi/\sigma_1^<em>), (\pi/\sigma_2^</em>)</td>
<td>7.79</td>
<td>0.0002</td>
<td>5a&quot;-28a'(89.0%), 5a&quot;-32a&quot;(1.7%)</td>
</tr>
<tr>
<td>A''5 (\pi/\sigma_1^<em>), (\pi/\sigma_2^</em>)</td>
<td>8.00</td>
<td>0.0041</td>
<td>4a&quot;-25a'(92.9%), 4a&quot;-37a&quot;(1.2%)</td>
</tr>
<tr>
<td>tHQA</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A'1 (\pi_1/\pi_1^<em>), (\pi_2/\pi_2^</em>)</td>
<td>4.54</td>
<td>0.0670</td>
<td>6a*-7a&quot;(85.0%), 5a*-8a&quot;(10.7%)</td>
</tr>
<tr>
<td>A'2 (\pi_1/\pi_1^<em>), (\pi_2/\pi_2^</em>)</td>
<td>6.16</td>
<td>0.2192</td>
<td>6a*-8a&quot;(80.3%), 5a*-7a&quot;(12.6%)</td>
</tr>
<tr>
<td>A'3 (\pi_1/\pi_1^<em>), (\pi_2/\pi_2^</em>)</td>
<td>7.15</td>
<td>0.7593</td>
<td>5a&quot;-7a&quot;(80.6%), 6a*-8a&quot;(9.3%)</td>
</tr>
<tr>
<td>A'4 (\pi_1/\pi_1^<em>), (\pi_2/\pi_2^</em>)</td>
<td>7.42</td>
<td>0.2784</td>
<td>5a&quot;-8a&quot;(62.9%), 4a&quot;-7a&quot;(21.9%)</td>
</tr>
<tr>
<td>A''5 (\sigma_{1H, n_A}/\sigma_{A}, \sigma_{2H, n_A}/\sigma_{A}^*)</td>
<td>7.57</td>
<td>0.0734</td>
<td>28a'-29a'(79.2%), 27a'-29a'(14.1%)</td>
</tr>
<tr>
<td>A''1 (\pi/\sigma_{1H}^<em>), (\pi/\sigma_{A}^</em>)</td>
<td>5.95</td>
<td>0.00001</td>
<td>6a&quot;-30a'(75.0%), 6a&quot;-29a'(11.3%)</td>
</tr>
<tr>
<td>A''2 (\pi/\sigma_{A}^<em>), (\pi/\sigma_{1H}^</em>)</td>
<td>6.13</td>
<td>0.00008</td>
<td>6a&quot;-29a'(73.3%), 6a&quot;-30a'(12.0%)</td>
</tr>
<tr>
<td>A''3 (\pi/\sigma_{2H}^<em>\sigma_{A}^</em>), (\pi/\sigma_{1H}^<em>\sigma_{A}^</em>)</td>
<td>6.88</td>
<td>0.000004</td>
<td>6a&quot;-31a'(61.9%), 6a&quot;-32a'(21.9%)</td>
</tr>
<tr>
<td>A''4 (\pi/\sigma_{2H}^<em>\sigma_{A1}^</em>), (\pi/\sigma_{1H}^<em>\sigma_{A2}^</em>)</td>
<td>7.54</td>
<td>0.0003</td>
<td>6a&quot;-33a'(51.8%), 6a&quot;-32a'(31.5%)</td>
</tr>
<tr>
<td>A''5 (\pi/\sigma_{A1}^<em>), (\pi/\sigma_{A2}^</em>)</td>
<td>7.89</td>
<td>0.0024</td>
<td>5a&quot;-29a'(69.0%), 5a&quot;-31a'(17.8%)</td>
</tr>
<tr>
<td></td>
<td>cHQ-A2</td>
<td></td>
<td>tHQ-A2</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------------------------------------------------------</td>
<td>-------</td>
<td>------------------------------------------------------------------------</td>
</tr>
<tr>
<td>A'1</td>
<td>(π/π₁⁺),(π₂/π₂⁺)</td>
<td>4.46</td>
<td>7a&quot;-8a&quot;(85.1%),6a&quot;-9a&quot;(9.3%)</td>
</tr>
<tr>
<td>A'2</td>
<td>(π/π₁⁺),(π₂/π₂⁺)</td>
<td>6.09</td>
<td>7a&quot;-9a&quot;(78.4%),6a&quot;-8a&quot;(11.2%)</td>
</tr>
<tr>
<td>A'3</td>
<td>(π/π₁⁺),(π₂/π₂⁺)</td>
<td>7.11</td>
<td>6a&quot;-8a&quot;(79.3%),7a&quot;-9a&quot;(7.2%)</td>
</tr>
<tr>
<td>A'4</td>
<td>(π/π₁⁺),(π₂/π₂⁺)</td>
<td>7.45</td>
<td>6a&quot;-9a&quot;(78.8%),7a&quot;-8a&quot;(8.3%)</td>
</tr>
<tr>
<td>A'5</td>
<td>(π₁⁺,n₁/σ₁⁺),(n₂,π₂⁺/σ₂⁺)</td>
<td>7.53</td>
<td>31a'-34a' (42.7%), 32'-33a' (35.6%)</td>
</tr>
<tr>
<td>A'1</td>
<td>(π/π₁⁺),(π₂/π₂⁺)</td>
<td>4.64</td>
<td>6a&quot;-7a&quot;(85.4%), 5a&quot;-6a&quot;(12.3%)</td>
</tr>
<tr>
<td>A'2</td>
<td>(π/π₁⁺),(π₂/π₂⁺)</td>
<td>6.25</td>
<td>5a&quot;-7a&quot;(79.9%), 4a&quot;-6a&quot;(15.5%)</td>
</tr>
<tr>
<td>A'3</td>
<td>(π/π₁⁺),(π₂/π₂⁺)</td>
<td>7.20</td>
<td>4a&quot;-6a&quot;(79.8%), 5a&quot;-7a&quot;(12.8%)</td>
</tr>
<tr>
<td>A'4</td>
<td>(π/π₁⁺),(π₂/π₂⁺)</td>
<td>7.47</td>
<td>4a&quot;-7a&quot;(81.0%), 5a&quot;-6a&quot;(10.5%)</td>
</tr>
<tr>
<td>A'5</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>7.73</td>
<td>3a&quot;-6a&quot;(94.2%), 1a&quot;-6a&quot;(2.0%)</td>
</tr>
<tr>
<td>A'1</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>6.12</td>
<td>5a&quot;-25a'(85.7%), 2a&quot;-25a'(4.2%)</td>
</tr>
<tr>
<td>A'2</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>6.18</td>
<td>5a&quot;-26a'(86.6%), 3a&quot;-25a'(4.7%)</td>
</tr>
<tr>
<td>A'3</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>7.03</td>
<td>5a&quot;-27a'(85.5%), 5a&quot;-28a'(2.3%)</td>
</tr>
<tr>
<td>A'4</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>7.87</td>
<td>5a&quot;-28a'(82.0%), 5a&quot;-31a'(6.8%)</td>
</tr>
<tr>
<td>A'5</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>7.99</td>
<td>4a&quot;-26a'(83.3%), 4a&quot;-27a'(9.3%)</td>
</tr>
<tr>
<td>A'1</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>4.55</td>
<td>6a&quot;-7a&quot;(85.4%), 5a&quot;-8a&quot;(10.9%)</td>
</tr>
<tr>
<td>A'2</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>6.16</td>
<td>6a&quot;-8a&quot;(80.6%), 5a&quot;-7a&quot;(13.0%)</td>
</tr>
<tr>
<td>A'3</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>7.15</td>
<td>5a&quot;-7a&quot;(79.8%), 6a&quot;-8a&quot;(9.7%)</td>
</tr>
<tr>
<td>A'4</td>
<td>(π/π₁⁺),(π₂/π⁺)</td>
<td>7.42</td>
<td>5a&quot;-8a&quot;(66.2%), 4a&quot;-7a&quot;(18.1%)</td>
</tr>
<tr>
<td>A'5</td>
<td>(π₁⁺,n₁,π₂⁺/σ₂⁺),(n₂,π₁⁺,π₂⁺/σ₂⁺)</td>
<td>7.57</td>
<td>28a'-29a'(78.3%), 27a'-29a'(15.0%)</td>
</tr>
<tr>
<td>A'1</td>
<td>(π/π⁺)</td>
<td>5.91</td>
<td>6a&quot;-30a'(85.0%), 4a&quot;-30a'(3.3%)</td>
</tr>
<tr>
<td>A'2</td>
<td>(π/σ₁⁺),(π₂/σ⁺)</td>
<td>6.07</td>
<td>6a&quot;-29a'(79.9%), 6a&quot;-31a'(6.7%)</td>
</tr>
<tr>
<td>Configuration</td>
<td>Energy</td>
<td>p-value</td>
<td>Percentages</td>
</tr>
<tr>
<td>---------------</td>
<td>--------</td>
<td>---------</td>
<td>-------------</td>
</tr>
<tr>
<td>A'3(π/σ_{H1}^<em>, σ_{A1}^</em>) (\sigma_{A2}^<em>) (\pi/\sigma_{H2}^</em>)</td>
<td>6.87</td>
<td>0.00001</td>
<td>6a&quot;-31a'(55.6%), 6a&quot;-32a'(19.1%)</td>
</tr>
<tr>
<td>A'4(π/σ_{H1}^<em>, σ_{A1}^</em>) (\sigma_{A2}^*)</td>
<td>7.59</td>
<td>0.000005</td>
<td>6a&quot;-32a'(56.7%), 6a&quot;-33a'(24.5%)</td>
</tr>
<tr>
<td>A'5(π/σ_{A1}^*)</td>
<td>7.77</td>
<td>0.00024</td>
<td>5a&quot;-30a'(44.0%), 5a&quot;-29a'(33.4%)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Energy</th>
<th>p-value</th>
<th>Percentages</th>
</tr>
</thead>
<tbody>
<tr>
<td>cHQ-A2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A'1(π/π_{1}^<em>) (\pi/\sigma_{H}^</em>)</td>
<td>4.47</td>
<td>0.0690</td>
<td>7a&quot;-8a'(86.2%), 6a&quot;-9a'(9.9%)</td>
</tr>
<tr>
<td>A'2(π/π_{1}^<em>) (\pi/\sigma_{A}^</em>)</td>
<td>6.10</td>
<td>0.2518</td>
<td>7a&quot;-8a'(78.6%), 7a&quot;-9a'(7.8%)</td>
</tr>
<tr>
<td>A'3(π/π_{1}^<em>) (\pi/\sigma_{A}^</em>)</td>
<td>7.10</td>
<td>0.8155</td>
<td>6a&quot;-8a'(78.6%), 7a&quot;-9a'(7.8%)</td>
</tr>
<tr>
<td>A'4(π/π_{1}^<em>) (\pi/\sigma_{A}^</em>)</td>
<td>7.45</td>
<td>0.4197</td>
<td>6a&quot;-8a'(81.2%), 7a&quot;-9a'(7.9%)</td>
</tr>
<tr>
<td>A'5(π/π_{1}^<em>) (\pi/\sigma_{A}^</em>)</td>
<td>7.45</td>
<td>0.0119</td>
<td>5a&quot;-8a'(90.1%), 3a&quot;-8a'(2.2%)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CTC</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A'1(π/π_{1}^<em>) (\pi/\sigma_{H}^</em>)</td>
<td>4.97</td>
<td>0.0414</td>
<td>5a&quot;-6a'(71.4%), 4a&quot;-7a'(23.3%)</td>
</tr>
<tr>
<td>A'2(π/π_{1}^<em>) (\pi/\sigma_{A}^</em>)</td>
<td>6.17</td>
<td>0.0703</td>
<td>5a&quot;-7a'(69.5%), 4a&quot;-6a'(21.5%)</td>
</tr>
<tr>
<td>A'3(π/π_{1}^<em>) (\pi/\sigma_{A}^</em>)</td>
<td>6.99</td>
<td>0.4753</td>
<td>4a&quot;-6a'(62.6%), 5a&quot;-7a'(19.4%)</td>
</tr>
<tr>
<td>A'4(π/π_{1}^<em>) (\pi/\sigma_{A}^</em>)</td>
<td>7.07</td>
<td>0.6516</td>
<td>4a&quot;-7a'(61.2%), 5a&quot;-6a'(16.4%)</td>
</tr>
<tr>
<td>A'5(π/π_{1}^<em>) (\pi/\sigma_{A}^</em>)</td>
<td>8.55</td>
<td>0.0895</td>
<td>3a&quot;-6a'(84.8%), 4a&quot;-7a'(4.4%)</td>
</tr>
<tr>
<td>A&quot;1(π/σ_{A1}^<em>) (\pi/\sigma_{A1}^</em>)</td>
<td>5.70</td>
<td>0.0000</td>
<td>7a&quot;-33a'(82.8%), 7a&quot;-35a'(7.8%)</td>
</tr>
<tr>
<td>A&quot;2(π/σ_{A1}^<em>) (\pi/\sigma_{A1}^</em>)</td>
<td>5.84</td>
<td>0.000002</td>
<td>7a&quot;-34a'(89.2%), 4a&quot;-34a'(3.1%)</td>
</tr>
<tr>
<td>A&quot;3(π/σ_{A1}^<em>) (\pi/\sigma_{A1}^</em>)</td>
<td>6.70</td>
<td>0.0000</td>
<td>7a&quot;-35a'(60.9%), 7a&quot;-37a'(13.8%)</td>
</tr>
<tr>
<td>A&quot;4(π/σ_{A1}^<em>) (\pi/\sigma_{A1}^</em>)</td>
<td>7.36</td>
<td>0.0000</td>
<td>7a&quot;-37a'(73.8%), 7a&quot;-39a'(7.3%)</td>
</tr>
<tr>
<td>A&quot;5(π/σ_{A1}^<em>) (\pi/\sigma_{A1}^</em>)</td>
<td>7.52</td>
<td>0.0016</td>
<td>6a&quot;-33a'(67.9%), 6a&quot;-35a'(18.6%)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Energy</th>
<th>p-value</th>
<th>Percentages</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTC-A</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A'1(π/π_{1}^<em>) (\pi/\sigma_{H}^</em>)</td>
<td>4.91</td>
<td>0.0495</td>
<td>6a&quot;-7a'(72.3%), 5a&quot;-8a'(21.8%)</td>
</tr>
<tr>
<td>A'2(π/π_{1}^<em>) (\pi/\sigma_{H}^</em>)</td>
<td>6.05</td>
<td>0.0824</td>
<td>6a&quot;-8a'(72.5%), 5a&quot;-7a'(18.6%)</td>
</tr>
<tr>
<td>A'3(π/π_{1}^<em>) (\pi/\sigma_{H}^</em>)</td>
<td>6.90</td>
<td>0.4771</td>
<td>5a&quot;-7a'(72.0%), 6a&quot;-8a'(16.8%)</td>
</tr>
<tr>
<td>A'4(π/π_{1}^<em>) (\pi/\sigma_{H}^</em>)</td>
<td>6.96</td>
<td>0.6549</td>
<td>5a&quot;-8a'(66.0%), 6a&quot;-7a'(17.3%)</td>
</tr>
<tr>
<td>Reaction</td>
<td>k</td>
<td>2k</td>
<td>Percentages</td>
</tr>
<tr>
<td>----------</td>
<td>---</td>
<td>----</td>
<td>-------------</td>
</tr>
<tr>
<td>A'5(σ_H1,n_H1,n_A1/σ_A*)</td>
<td>7.68</td>
<td>0.1149</td>
<td>28α'-29α'(78.0%), 27α'-29α'(14.9%)</td>
</tr>
<tr>
<td>A''1(π/σ_A*),(π/σ*)</td>
<td>6.13</td>
<td>0.0004</td>
<td>6α''-29α'(79.3%), 6α''-32α'(7.5%)</td>
</tr>
<tr>
<td>A''2(π/σ_H1,σ_A*),(π/σ_H2,σ_A*)</td>
<td>6.56</td>
<td>0.0001</td>
<td>6α''-30α'(55.5%), 6α''-32α'(24.7%)</td>
</tr>
<tr>
<td>A''3(π/σ_A*),(π/σ*)</td>
<td>7.14</td>
<td>0.0025</td>
<td>5α''-29α'(67.2%), 6α''-32α'(9.2%)</td>
</tr>
<tr>
<td>A''4(π/σ_H1,σ_A*),(π/σ_H2,σ_A*)</td>
<td>7.28</td>
<td>0.0006</td>
<td>6α''-32α'(40.1%), 6α''-30α'(17.3%)</td>
</tr>
<tr>
<td>A''5(π/σ_H1,σ_A*),(π/σ_H2,σ_A*)</td>
<td>7.57</td>
<td>0.000001</td>
<td>5α''-30α'(63.3%), 5α''-32α'(9.8%)</td>
</tr>
</tbody>
</table>

**CTC-A2**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>k</th>
<th>2k</th>
<th>Percentages</th>
</tr>
</thead>
<tbody>
<tr>
<td>A'1(π/π*),(π/π*)</td>
<td>4.84</td>
<td>0.0613</td>
<td>7α''-8α''(72.0%), 6α''-9α''(19.3%)</td>
</tr>
<tr>
<td>A'2(π/π*),(π/π*)</td>
<td>5.94</td>
<td>0.0995</td>
<td>7α''-9α''(70.5%), 6α''-8α''(17.6%)</td>
</tr>
<tr>
<td>A'3(π/π*),(π/π*)</td>
<td>6.79</td>
<td>0.4501</td>
<td>6α''-8α''(62.8%), 7α''-9α''(16.6%)</td>
</tr>
<tr>
<td>A'4(π/π*),(π/π*)</td>
<td>6.89</td>
<td>0.6681</td>
<td>6α''-9α''(61.1%), 7α''-8α''(12.3%)</td>
</tr>
<tr>
<td>A'5(σ_H1,n_H1,n_A1/σ_A*)</td>
<td>7.46</td>
<td>0.0562</td>
<td>32α''-34α''(74.4%), 32α''-33α''(10.8%)</td>
</tr>
<tr>
<td>A''1(π/σ_A*),(π/σ_A*)</td>
<td>5.77</td>
<td>0.00009</td>
<td>7α''-33α''(83.9%), 5α''-33α''(3.5%)</td>
</tr>
<tr>
<td>A''2(π/σ_A*),(π/σ_A*)</td>
<td>6.34</td>
<td>0.00003</td>
<td>7α''-34α''(57.7%), 7α''-35α''(14.2%)</td>
</tr>
<tr>
<td>A''3(π/σ_A*),(π/σ_A*),σ_A*)</td>
<td>6.82</td>
<td>0.0016</td>
<td>6α''-33α''(77.5%), 7α''-35α''(4.1%)</td>
</tr>
<tr>
<td>A''4(π/σ_H1,σ_A*),(π/σ_H2,σ_A*)</td>
<td>7.00</td>
<td>0.0011</td>
<td>7α''-36α''(33.0%), 7α''-35α''(31.3%)</td>
</tr>
<tr>
<td>A''5(π/σ_A*),(π/σ_H1,σ_A*)</td>
<td>7.39</td>
<td>0.00008</td>
<td>6α''-34α''(34.9%), 6α''-35α''(25.4%)</td>
</tr>
</tbody>
</table>
Table SM2

<table>
<thead>
<tr>
<th></th>
<th>tHQ</th>
<th>cHQ</th>
<th>CTC</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.71115</td>
<td>-1.19334</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>0.68016</td>
<td>-1.21508</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>1.39516</td>
<td>-0.02145</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>0.71115</td>
<td>1.19334</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>-0.68016</td>
<td>1.21508</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>-1.39515</td>
<td>0.02145</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-1.26154</td>
<td>-2.12838</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>1.26154</td>
<td>2.12838</td>
<td>0</td>
</tr>
<tr>
<td>O</td>
<td>2.76701</td>
<td>-0.10900</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>1.26154</td>
<td>2.12838</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-1.22038</td>
<td>2.15281</td>
<td>0</td>
</tr>
<tr>
<td>O</td>
<td>-2.76700</td>
<td>0.10900</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>3.12659</td>
<td>0.78545</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-3.12659</td>
<td>-0.78545</td>
<td>0</td>
</tr>
</tbody>
</table>

![Diagram of tHQ, cHQ, and CTC molecules]
<table>
<thead>
<tr>
<th></th>
<th>tHQ-A2</th>
<th>chQ-A2</th>
<th>CTC-A2</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-0.09389</td>
<td>1.38464</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>-1.26223</td>
<td>0.62370</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>-1.15551</td>
<td>-0.77039</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>0.09389</td>
<td>-1.38465</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>1.26223</td>
<td>-0.62370</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>1.15551</td>
<td>0.77039</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>2.05180</td>
<td>1.37928</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>0.17815</td>
<td>2.46438</td>
<td>0</td>
</tr>
<tr>
<td>O</td>
<td>-2.45551</td>
<td>1.28594</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-3.19298</td>
<td>0.63739</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-2.05180</td>
<td>-1.37928</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>0.17814</td>
<td>2.46439</td>
<td>0</td>
</tr>
<tr>
<td>O</td>
<td>2.45551</td>
<td>-1.28595</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>3.19298</td>
<td>-0.63739</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>4.88622</td>
<td>0.97262</td>
<td>0.81362</td>
</tr>
<tr>
<td>N</td>
<td>4.76508</td>
<td>0.38048</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>5.53823</td>
<td>-0.27525</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>4.88622</td>
<td>0.97262</td>
<td>-0.81362</td>
</tr>
<tr>
<td>H</td>
<td>-4.88622</td>
<td>-0.97261</td>
<td>0.81362</td>
</tr>
<tr>
<td>N</td>
<td>-4.76508</td>
<td>-0.38048</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-5.53823</td>
<td>0.27525</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-4.88622</td>
<td>-0.97261</td>
<td>0.81362</td>
</tr>
</tbody>
</table>

**Diagram:**
- tHQ-A2
- chQ-A2
- CTC-A2
<table>
<thead>
<tr>
<th></th>
<th>tHQ-A4</th>
<th>chQ-A4</th>
<th>CTC-A4</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>-3.05708</td>
<td>-2.27905</td>
<td>0</td>
</tr>
<tr>
<td>O</td>
<td>-2.65554</td>
<td>-1.36749</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>-1.29479</td>
<td>-1.43989</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>-0.57209</td>
<td>-0.24666</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-1.12202</td>
<td>0.68728</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>0.82056</td>
<td>0.67917</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>1.52644</td>
<td>-1.46134</td>
<td>0</td>
</tr>
<tr>
<td>O</td>
<td>2.88697</td>
<td>-1.53380</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>3.06883</td>
<td>-0.62288</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>0.80377</td>
<td>-2.65453</td>
<td>0</td>
</tr>
<tr>
<td>C</td>
<td>-0.58971</td>
<td>-2.64754</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>1.35375</td>
<td>-3.58844</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>3.49856</td>
<td>1.80918</td>
<td>0</td>
</tr>
<tr>
<td>N</td>
<td>4.12041</td>
<td>0.99921</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>4.72501</td>
<td>1.08737</td>
<td>0.81231</td>
</tr>
<tr>
<td>H</td>
<td>4.72501</td>
<td>1.08737</td>
<td>-0.81231</td>
</tr>
<tr>
<td>H</td>
<td>2.03807</td>
<td>3.99365</td>
<td>-0.81270</td>
</tr>
<tr>
<td>N</td>
<td>1.99730</td>
<td>3.89337</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>2.03807</td>
<td>3.99365</td>
<td>0.81270</td>
</tr>
<tr>
<td>H</td>
<td>1.07119</td>
<td>2.97654</td>
<td>0</td>
</tr>
<tr>
<td>O</td>
<td>-3.26661</td>
<td>-4.71022</td>
<td>0</td>
</tr>
<tr>
<td>N</td>
<td>-3.88880</td>
<td>-3.90052</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-4.48880</td>
<td>-3.98881</td>
<td>0.81235</td>
</tr>
<tr>
<td>H</td>
<td>-4.48880</td>
<td>-3.98881</td>
<td>-0.81235</td>
</tr>
<tr>
<td>H</td>
<td>-1.80628</td>
<td>-6.89535</td>
<td>-0.81272</td>
</tr>
<tr>
<td>N</td>
<td>-1.76627</td>
<td>-6.29110</td>
<td>0</td>
</tr>
<tr>
<td>H</td>
<td>-1.80628</td>
<td>-6.89535</td>
<td>0.81272</td>
</tr>
<tr>
<td>H</td>
<td>-0.84042</td>
<td>-5.87761</td>
<td>0</td>
</tr>
</tbody>
</table>